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NOTE TO USERS

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ADAPTIVE MODEL PREDICTIVE CONTROL OF A TWO-PHASE CHEMICAL REACTOR

TOMMASO GIOVANNI DEL BIANCO
DÉPARTEMENT DE GÉNIE CHIMIQUE
ÉCOLE POLYTECHNIQUE DE MONTRÉAL

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Ce mémoire intitulé :

ADAPTIVE MODEL PREDICTIVE CONTROL
OF A TWO-PHASE CHEMICAL REACTOR

présenté par : DEL BIANCO Tommaso Giovanni
en vue de l'obtention du diplôme de : Maîtrise ès sciences appliquées
a été dûment accepté par le jury d'examen constitué de :

M. SRINIVASAN Balasubrahmanyan, Ph.D., président
M. PERRIER Michel, Ph.D., membre et directeur de recherche
M. GENDRON Sylvain, Ph.D., membre

For Betrand

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RÉSUMÉ

L'objectif de ce projet consiste à améliorer la performance du contrôle d'un réacteur chimique biphasique. L'application considérée est une simplification du procédé Tennessee Eastman et elle présente les mêmes comportements et les mêmes défis. Des travaux antérieurs sur la même application ont montré qu'une stratégie de contrôle classique fonctionne assez bien mais qu'elle donne une piètre performance. Par contre, l'utilisation de stratégies de contrôle avancées peut être problématique.
La nature multivariable et contrainte de ce problème porte à l'utilisation des stratégies de contrôle par MPC (Model Predictive Control). Les fortes non-linéaritées et les conditions d'opérations variables suggèrent l'utilisation des techniques d'adaptation de modèle. Trois stratégies différentes sont utilisées et comparées.

Premièrement, une stratégie mixte a été utilisée. Cette stratégie mixte est représentée par deux contrôleurs PI classiques et un contrôleur MPC linéaire monovariable. Une amélioration appréciable de performance est obtenue grâce à la nature prédictive du contrôleur utilisé, mais des limitations sont dues à l'approche décentralisée et aux phénomènes de saturation de valves.

Une approche centralisée par MPC linéaire a été utilisée pour diminuer l'effet de ces limitations. L'augmentation de la performance de contrôle avec cette approche est très importante dans les cas de changements de points de consigne et dans le cas de rejet des perturbations. Néanmoins, des difficultés ont été rencontrées en termes de stabilité et de réglage. Ces problèmes sont dus à la présence des contraintes sur les entrées et sur les sorties, et aux non linéarités du système. En particulier le changement de signe d'une des fonctions de transfert est à l'origine de certains problèmes.

L'utilisation des techniques d'adaptation de modèle a été ajoutée à la stratégie de contrôle conçue. En particulier la technique de Model Weighting Adaptation (MWA) a

été choisie à cause de sa simplicité et de sa rapidité de convergence. Deux approches ont été utilisées : premièrement, seulement la fonction de transfert présentant le changement de signe du gain a été adaptée et par la suite le modèle complet de la pression du réacteur a été adapté. Les deux approches ont montrés des graves problèmes d'identification du système pendant des tests préliminaires. Si la boucle d'adaptation du modèle est fermée, l'approche monovariable garantit une performance comparable, ou légèrement meilleure que le MPC a modèle fixe. Par contre, l'approche multivariable dégrade la performance. Par la suite, un algorithme récursif de moindres carrés (Recursive Least Square, RLS) a été utilisé pour valider les résultats de l'algorithme MWA monovariable.

ABSTRACT

The goal of this work is to improve control performance of a two-phase chemical reactor. The application considered is a simplification of the well known Tennesee Eastman challenge problem and it shows the same behavior and challenges. Previous work on this application showed that classical control strategies work fairly well but with poor performance while advanced control techniques result to be problematic.
The multivariable and constrained nature of the problem leads to the use of a Model Predictive Control (MPC) algorithm. Large nonlinearities and varying operating conditions suggest the possibility of using model adaptation techniques. Three strategies were implemented and compared.

First a mixed multiloop strategy was used. This strategy uses two classic PI controllers and one single-input single-output linear MPC. Performance improvement is obtained due to the predictive nature of the controller used, but major limitations are still unavoidable because of the decentralized strategy used and the occurrence of valve saturation phenomena.

In order to overcome these difficulties a fully centralized linear MPC approach was used. Performance improvement with this approach is very important both in setpoint changes and in disturbance rejection. Nevertheless some difficulties were encountered with respect to stability and tuning. The reasons for such difficulties were identified in the input and output constraints and in the high degree of nonlinearity. In particular, the gain sign inversion of one of the transfer functions was the cause of many problems.

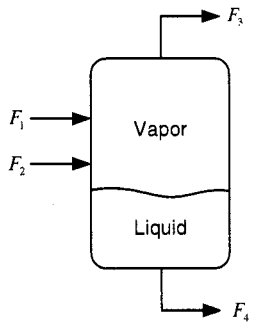
Model adaptation techniques were identified as a possible solution to this problem. Model Weighting Adaptation (MWA) was considered to be particularly well-suited for this application because of its simplicity and rapidity of convergence. Two approaches were considered: the adaptation of only the transfer function presenting the gain sign

inversion (SISO MWA) and the adaptation of the pressure dynamic model (MISO MWA). Both approaches showed serious identifiability problem during preliminary tests. When the adaptation loop is closed, SISO MWA guarantees performance that is comparable, if not better than the fixed-model MPC. On the contrary, MISO MWA results in a slight performance degradation. A classic Recursive Least Square (RLS) approach was also used to validate the results obtained with the SISO MWA.

CONDENSÉ EN FRANÇAIS

Description du problème

L'objectif de ce projet consiste à améliorer la performance de contrôle d'un réacteur non linéaire bi-phasique (Ricker, 1993). Le problème considéré est une simplification du procédé Tennessee Eastman (Downs et Vogel, 1993) et il garde les mêmes caractéristiques et les mêmes défis. Un schéma du réacteur est fourni à la figure suivante :



Le réacteur produit le composant D liquide et non volatil à partir de deux réactifs gazeux, non condensables, selon la réaction suivante. Une impureté (B) est aussi présente dans l'alimentation principale (F_1).

$$A_{gas} + C_{gas} \longrightarrow D_{liquid}$$

Pour rendre le système stable en boucle ouverte, le réacteur est équipé d'un contrôleur proportionnel sur niveau qui manipule le courant liquide.

Le système est caractérisé par 8 états (les masses des 4 composants et les positions des 4 vannes); les entrées du système sont données par les ouvertures des vannes 1, 2 et 3 et le point de consigne du niveau du liquide; les sorties (10) comprennent des mesures des débits, de composition et de pression.

Des contraintes sont présentes sur les variables manipulées (0-100%), sur la pression (limite de *shut-down*) et sur le niveau du liquide (0-100%). Une autre caractéristique remarquable est donnée par les fortes non-linearitées du système; en particulier la fonction de transfert entre la pression et l'alimentation en A pur (F_2) présente un changement de signe de gain. Ces deux aspects (contraintes et non linéarités) représentent les deux caractéristiques les plus importantes de ce problème.

À la suite des considérations de contrôlabilité et d'autorité de contrôle, le taux de production (F_4), la pression (P), la fraction molaire de A (y_{A3}) et le niveau du liquide (liq) sont choisies comme variables contrôlées.

De plus, Ricker (1993) propose des scénarios afin de tester la performance des différentes stratégies de contrôle. Ces scénarios incluent des changements de point de consigne sur le taux de production et sur la composition, ainsi que des perturbations sur la composition de l'alimentation et sur la cinétique de réaction.

Différentes stratégies de contrôle sont présentées dans Ricker (1993). Une approche PI décentralisée marche assez bien mais souffre en performance; une stratégie par MPC (Model Predictive Control) présente des sérieux problèmes de stabilité et une stratégie MPC décentralisée donne une performance comparable, sinon meilleure que l'approche par contrôleurs PI.

Vue la nature multivariable et contrainte du problème, trois différentes stratégies de contrôle basées sur une approche par MPC seront utilisées et comparées. Les fortes non-linearités et les conditions d'opération variables suggèrent la possibilité d'utiliser des techniques d'adaptation de modèle.

Commande par MPC

La commande par MPC regroupe nombreux algorithmes très différents mais trois ingrédients de base peuvent être identifiés (Bequette (2002)). Il s'agit d'un algorithme basé sur un modèle du procédé, il est 'optimal' et il est implanté d'une façon à 'horizon reculant' (*receding horizon*).

Les actions de contrôle sont calculées comme le résultat de l'optimisation des différences entre la trajectoire de référence et la sortie prédite du procédé plus des termes de pénalité sur les mouvements des entrées. Ceci garantit une solution 'optimale'. Pour limiter l'effet des erreurs de prédictions, une seule action de contrôle est appliquée et à chaque échantillonnage la procédure est répétée en tenant compte de l'erreur commis.

La caractéristique remarquable de ces algorithmes est la capacité de traiter des systèmes multivariables et avec contraintes (Ogunnaike, 1994).

Stratégie Mixte

Comme anticipé, une stratégie mixte a été essayée. Celle-ci consiste de l'approche PI décentralisée de Ricker (1993) où un des contrôleurs est remplacé par un MPC monovariable. Suite aux propriétés du MPC de traiter les contraintes, cette approche est appliquée à la boucle de la pression du réacteur. Le modèle fournis au contrôleur a été estimé grâce à un test de -5% sur la valve de purge.

Dans ce cas le réglage du contrôleur MPC ne pose pas de problèmes particuliers à cause du faible nombre de paramètres à choisir et à cause de l'approche monovariable.

L'utilisation de cette stratégie mixte pendant les scénarios proposés garantit une amélioration appréciable de la performance, dont des exemples sont fournis aux figures suivantes. Néanmoins des limitations sont dues à l'approche décentralisée et à la saturation des valves.

MPC Multivariable

Pour faire face aux problèmes rencontrés avec l'approche précédente, une stratégie par MPC multivariable est utilisée. Celle-ci est appliquée au système complet de 4 entrées et 4 sorties. Comme pour le cas précédent le modèle utilisé a été trouvé grâce a des *steps* de ±5% sur les entrées du système.

Dans ce cas ci la difficulté principale est donnée par le réglage du contrôleur qui comprend le choix de 12 paramètres après certaines simplifications. En particulier le choix des poids pour les variables manipulées et contrôlées est crucial. Pour simplifier cette procédure, les poids pour les entrées sont calculés selon l'influence 'globale' de chaque entrée sur les sorties pondérées, c'est-à-dire selon la diagonale principale de la matrice suivante :

$$\Omega = \underline{\underline{\beta}}^T \underline{\underline{\Lambda}}_y \underline{\underline{\beta}}$$

ou $\underline{\underline{\beta}}$ est la 'matrice dynamique' du système (Ogunnaike, 1994).

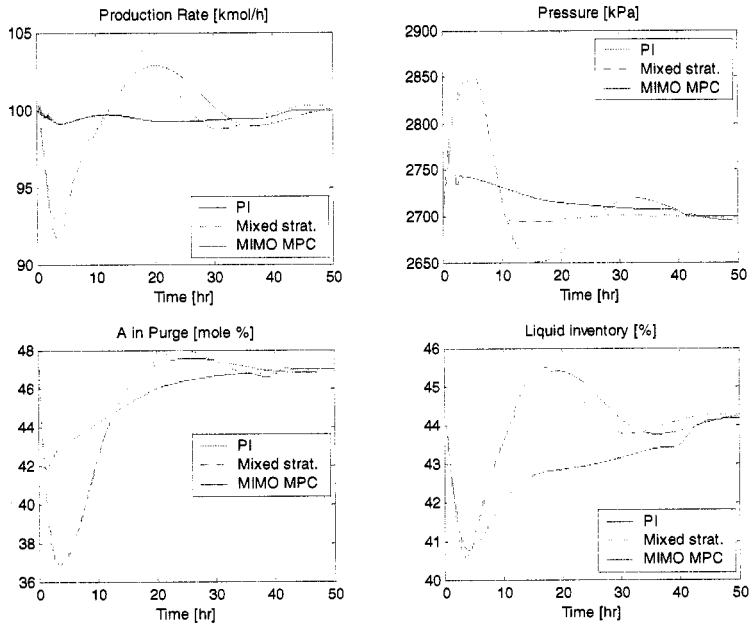
Les poids pour les entrées ont du être choisis non seulement à partir des considérations économiques et de priorité, mais ils ont été dictés aussi par des problèmes de stabilité. La cause de ces problèmes a été identifiée dans le contraintes du système et dans l'inversion du signe du gain caractéristique de la fonction de transfert P/u_2. Les autres paramètres sont relativement faciles à choisir et ils n'ont pas des conséquences importantes sur la performance.

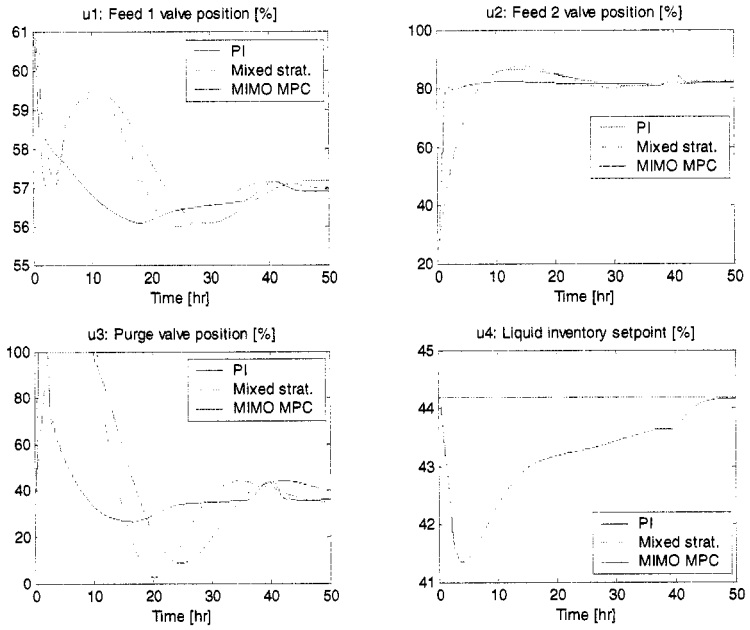
Résultats

Il est difficile de montrer et discuter d'une façon brève et exhaustive les résultats trouvés avec les deux premiers exemples. Ici deux scénarios sont montrés à titre d'exemple.

Dans le cas du scénario 1, une perturbation sur la composition de l'alimentation affecte le système. Il est évident que la stratégie mixte améliore la trajectoire suivie par la pression sans variations appréciables sur les autres variables contrôlées. Cependant l'amélioration de performance est fortement limitée par la saturation de u_3 pendant les premières 10 heures.

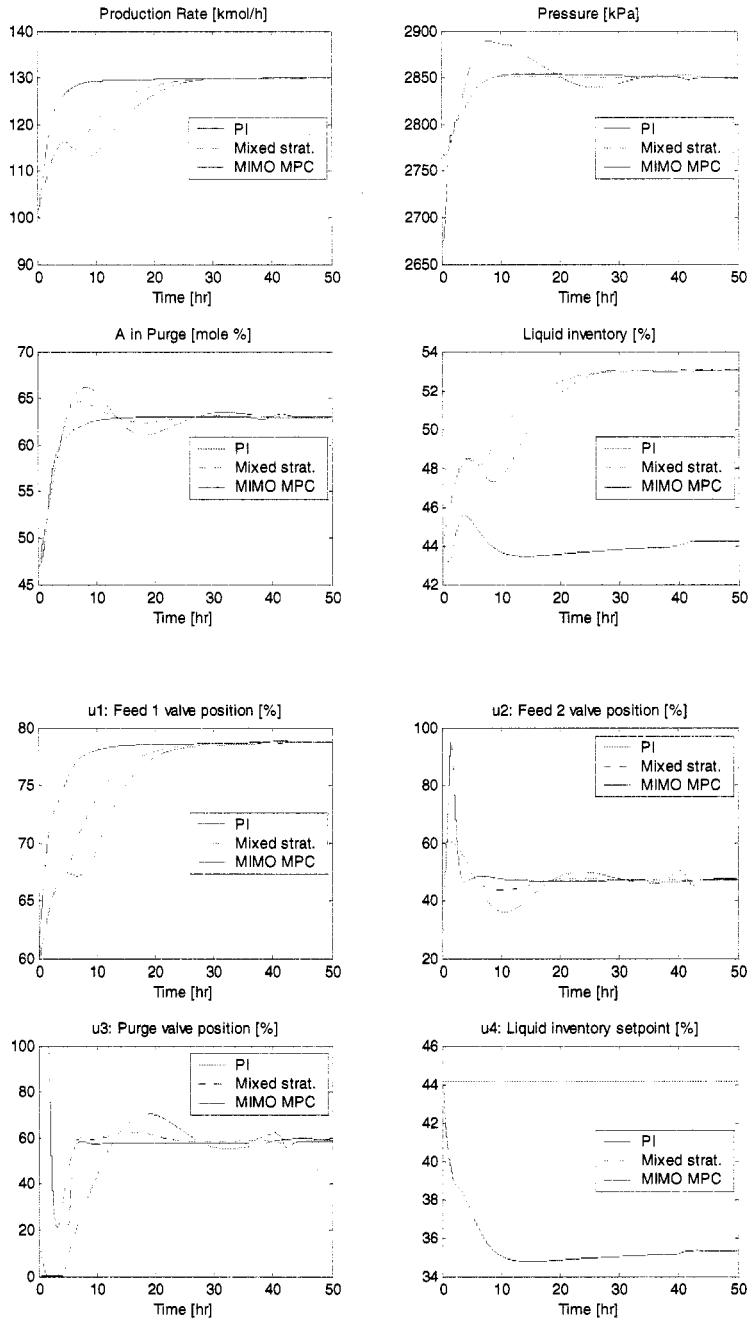
La stratégie par MPC multivariable apporte une grande amélioration pour toutes les variables contrôlées et ce résultat est obtenu grâce à une manipulation plus agressive et synergique des entrées du système.





Le scénario 2 offre un bon exemple de l'amélioration possible dans le cas d'un changement de point de consigne. Comme pour le cas précèdent, la stratégie mixte apporte une bonne amélioration seulement sur la trajectoire de la pression grâce à une manipulation rapide de u_3.

La stratégie par MPC centralisé conduit le système au nouveau point de consigne rapidement et sans oscillations ni dépassement. Ce résultat est possible grâce à la nature prédictive du contrôleur MPC.



La stratégie multivariable proposée apporte une amélioration très importante de la performance. Les raisons d'un tel succès résident dans l'approche multivariable qui permet une synergie des actions de contrôle. De plus la nature prédictive de

l'algorithme permet une manipulation des entrés 'optimale', c'est-à-dire visant à la minimisation de l'écart entre sorties et trajectoire de référence. De plus la capacité du MPC de traiter avec les contraintes améliore ultérieurement la performance.
Néanmoins, la performance est limitée par les fortes non-linearités du système qui entraînent une erreur remarquable entre la prédiction et le comportement réel du système. Cela a imposé certaines valeurs du réglage et limité la marge d'amélioration. En particulier le changement de signe de la fonction de transfert P/u_2 peut être problématique.
Tout cela suggère l'utilisation des techniques d'adaptation du modèle utilisé par le contrôleur.

Adaptation du Modèle

Les difficultés rencontrées avec l'approche précédente sont en général causées par l'erreur entre la prédiction et le comportement réel du système. Cela suggère l'utilisation des techniques d'adaptation de modèle.
L'algorithme utilisé est le Model Weighting Adaptation (MWA) à cause de sa simplicité et de sa rapidité de convergence. Deux approches sont considérées : premièrement seulement la fonction qui présente le changement de signe est adaptée; ensuite, à cause des problèmes rencontrés, l'adaptation se fait sur les trois fonctions de transfert qui contribuent le plus aux variations de pression.
Un algorithme RLS est aussi utilisé pour comparer les résultats obtenus avec le MWA monovariable.

Model Weighting Adaptation

L'algorithme de Model Weighting Adaptation est analysé en détail dans Gendron (1998). Il s'agit d'une approche très simple et puissante, utilisée dans l'industrie. Le modèle du système est calculé comme la composition linéaire d'un nombre fini de

modèles simples. La famille des modèles est en général composée par des fonctions de premier ordre avec retard avec des plages prédéfinies pour les gains et pour les retards. Le poids de chaque membre de la famille $w_i(t)$ est calculé à partir de l'erreur que ce membre entraîne sur la réponse du système, c'est-à-dire :

$$w_i(t) = \frac{\left(\mu + \left\|e_i(t)\right\|_{2,\lambda}^2\right)^{-1}}{\sum\left(\mu + \left\|e_i(t)\right\|_{2,\lambda}^2\right)^{-1}}$$

De plus, une mesure de la précision de l'identification obtenue est disponible *on line*. Celle-ci est représentée par l'uniformité' (*'flatness'*) de la matrice des poids et elle est facilement calculée par:

$$W(t) = \sum_i \sqrt{w_i(t)}$$

Des faibles valeurs de W impliquent une bonne discrimination entre les membre de la famille et par conséquent une bonne identification.

Gendron (1998) présente une version monovariable (SISO) de l'algorithme. Dans ce projet, une extension au cas multivariable a été élaborée. Celle-ci se base sur plusieurs familles de modèles, une pour chaque fonction de transfert à identifier; les poids globaux sont calculés a partir des toutes les combinaisons possibles des membres de différentes familles.

MWA Monovariable

Si seulement la fonction de transfert reliant u_2 à P est à adapter, il est nécessaire d'isoler la contribution de u_2 sur la variation totale de pression. L'approche plus simple

est de soustraire la contribution de u_1 et de u_3 selon le modèle nominal utilisé par le MPC à model fixe (u_4 peut être négligé) :

$$P_2' = P' - g_{P,1}u_1' - g_{P,3}u_3' = g_{P,2}u_2'$$

Des tests préliminaires sont effectués avec la boucle d'adaptation ouverte pour tester l'habilité de l'algorithme de bien identifier la fonction de transfert visée. La comparaison des gains identifiés et réels montre que l'objectif préfixé n'est pas atteint. La cause de cela est à rechercher dans l'utilisation de g_{P1} et g_{P3} fixes et égaux au modèle nominal, qui entraîne des grandes erreurs sur l'estimation de la contribution de u_1 et u_3 et, par conséquent, sur le gain de g_{P2}.

Malgré les difficultés rencontrées la boucle d'adaptation du modèle a été fermée et les scénarios proposés dans Ricker (1993) ont été testés. La performance obtenue est comparable, sinon meilleure que celle obtenue avec le MPC multivariable à modèle fixe. Les résultats de cette approche ne sont pas montrés dans ce condensé pour des raisons de brévité. Le lecteur est invité à faire référence au corps de ce travail.

MWA Multivariable

La réponse naturelle aux problèmes rencontrés est d'adapter les trois fonctions de transfert (g_{P1}, g_{P2} et g_{P3}) en même temps. Les plages des gains et des retards pour les trois familles de modèles sont spécifiées selon les réponses observées à différentes conditions d'opération.

Similairement au cas précédent, des tests préliminaires sont effectués avec la boucle d'adaptation ouverte. Les résultats de cette procédure montrent que l'algorithme MWA multivariable n'est pas capable d'identifier correctement le modèle dynamique de la pression. En particulier, les gains identifiés se situent toujours en correspondance du gain moyen de chaque famille et les valeurs de l'uniformité sont toujours très élevées.

Ces deux faits, montrent que l'algorithme n'est pas capable de discriminer entre les membres de chaque famille et le modèle résultant correspond à une combinaison 'uniforme' des modèles possibles.

Les raisons de ces problèmes sont identifiés dans : 1) la proximité des constantes de temps des trois fonctions de transfert; 2) la manipulation simultanée des entrées du système; 3) la disposition des trois plages des gains qui détermine une superposition de la plage des gains possibles de g_{P2} avec les plages de g_{P1} et g_{P3}. Les deux derniers facteurs sont à considérer les plus influents.

Malgré les difficultés rencontrées, des tests avec la boucle d'adaptation du modèle fermé a été faits pour les scénarios proposés dans Ricker (1993). La performance résultante est acceptable, mais inférieure à celle du MPC à modèle fixe. Les différences majeures sont en terme d'oscillations et de déviation du point de consigne. Pour une discussion des résultats de cette approche le lecteur est invité à faire référence au corps de ce travail.

Méthode des Moindre Carrés

Un algorithme classique de moindres carrés (Recursive Least Squares, RLS) a été utilisé pour comparer les résultats obtenus avec l'approche MWA. L'algorithme traditionnel avec facteur d'oubli a été choisi.

L'implémentation dans le cas monovariable (g_{P2} seulement) donne des résultats en boucle ouverte qui confirment dans une certaine mesure les valeurs trouvées avec l'algorithme MWA. Même dans ce cas l'utilisation de g_{P1} et g_{P3} fixes détermine une sous-estimation ou une sur-estimation de la contribution de u_2 ; de plus, la rapidité de convergence du RLS pose des problèmes additionnels.

Par contre, l'approche multivariable du RLS donne des valeurs des gains pour g_{P1}, g_{P2} et g_{P3} qui ne sont pas raisonnables : soit des valeurs trop élevées soit des signes physiquement impossibles. Les raisons de ces problèmes, sont environ les mêmes que pour l'algorithme MWA, mais dans ce cas la manipulation simultanée des entrés du système joue un rôle encore plus important.

Conclusions et recommandations

Le but de ce projet était d'améliorer la performance du contrôle d'un réacteur biphasique représentant une simplification du procédé Tennessee Eastman. La nature multivariable et contrainte de ce problème conduit vers une approche par MPC, et l'utilisation des techniques d'adaptation de modèle est suggérée par les non-linearitées. Trois stratégies différentes ont été testées et comparées.

Une stratégie mixte apporte une amélioration mais des limitations sont encore présentes. Ces problèmes sont en partie résolus par une approche par MPC multivariable à modèle fixe qui entraîne une forte amélioration de la performance. Afin de réduire les effets des non-linearitées, des techniques d'adaptation de modèle ont été essayées, mais des problèmes d'identificabilité du système ont limité l'effet positif attendu.

Les points suivants résument les directions possibles des travaux futurs :

1. La possibilité d'appliquer une couche de supervision pourrait être considérée. Celle-ci aurait l'objectif de déterminer le nouveau point d'opération dans le cas ou le point original n'est plus possible.
2. L'application considérée a montré des graves problèmes d'identificabilité. Cet aspect pourrait être étudié plus en détail pour trouver des solutions aux difficultés rencontrées.

3. L'utilisation de techniques de contrôle non-linéaire, peut constituer une solution alternative à l'adaptation de modèle. En particulier une approche par MPC non-lineaire est vue comme un bon candidat.
4. L'application à l'étude est une simplification du problème Tennessee Eastman. Il serait intéressant d'étendre au procédé original les résultats obtenus avec le racteur biphasique consideré.
5. Dans ce travail l'algorithme MWA multivariable a été élaboré comme l'extension logique du cas monovariable. Des études plus détaillées pourraient traiter cet aspect en explorant les propriétés théoriques

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Abbreviations

DMC	Dynamic Matrix Control
FOPDT	First Order Plus Dead Time
GPC	General Predictive Control
MHC	Moving Horizon Control
MIMO	Multi-Input Multi-Output
MISO	Multi-Input Single-Output
MPC	Model Predictive Control
MWA	Model Weighting Adaptation
RGA	Relative Gain Array
RHC	Receding Horizon Control
RLS	Recursive Least Squares
SISO	Single-Input Single-Output
QDMC	Quadratic Dynamic Matrix Control
QP	Quadratic Programming
PAA	Parameter Adaptation Algorithm

Roman Letters

$A(q^{-1})$, $B(q^{-1})$	Polynomials in the q^{-1} operator
$a_i(t), b_i(t)$	Coefficients for the polynomials $A(q^{-1})$, $B(q^{-1})$
C	Instantaneous cost
$F(t)$	Adaptation gain
F_i	Stream 'i'
g_{P1}, g_{P2}, g_{P3}	Transfer function between Pressure and u_1, u_2, u_3
liq	Liquid inventory (%)
k_0	Pseudo-reaction constant

K	Gain matrix
K_C	Gain of the built-in P controller
K_{P1}, K_{P2}, K_{P3}	Gain of g_{P1}, g_{P2} and g_{P3}
M	Control horizon
N	Model length
N_i	Molar holdup of species 'i'
P	Prediction horizon
P_i, P	Partial pressure of species 'i', total pressure
q^{-1}	Backward shift operator $\left(q^{-1}(y(t)) = y(t-1)\right)$
R_D	Reaction rate
r_k	Reference trajectory at sampling time 'k'
S_f	Dynamic matrix for SISO systems
$s_1, s_2, \ldots s_N$	Coefficients for the step response model
T	Sampling time
u, x, y	System inputs, states and outputs
V_V, V_L, V_{TOT}	Vapor, liquid and total volume
w	Control action weighting
W	Weight map flatness
$w_{i,j}$	Weight for model family member 'i,j'
$\hat{y}_k$	Predicted output at sampling time 'k'
y_{ij}	Mole fraction of species 'i' in stream 'j'

Greek Letters

$\underline{\underline{\beta}}$	Dynamic matrix for MIMO systems
Δu_k	Incremental input at sampling time 'k'

$\varepsilon^0(t), \varepsilon(t)$	*A priori* and *a posteriori* prediction error
θ, $\hat{\theta}$	Vector of model parameters, estimate of
Λ	RGA matrix
Λ_y, Λ_u	Weighting matrices for system input and output
λ	Forgetting Factor
λ_u	Robustness scaling factor
$\lambda_{i,j}$	Elements of the RGA matrix
μ	Constant to prevent division by zero
$\tilde{\rho}_L$	Molar density of liquid
τ_V	Valve time constant
ϕ	Regressor, vector of the measurements
χ_i	Opening of valve 'i'

CHAPTER 1 Introduction

In the process industry it is extremely important to keep product specifications between given limits and to guarantee safety and operating constraints. For decades this task has been accomplished by classical PID controllers (Ogunnaike, 1994). However, process control research has always pushed towards more advanced control techniques, including model-based, nonlinear, and adaptive algorithms (Bequette, 2003). This research field can be very theoretical and newly developed techniques are tested on very simple systems. These are often single-input single-output systems with the assumption of known model.
Nevertheless, in order to be implementable in practice, a control strategy has to deal with 'real world' settings that include multivariable nonlinear problems, unknown models, constraints and disturbances affecting the system (Foss, 1973).

This explains the interest expressed by the process control community in having a benchmark process to test and compare different control strategies in situations close to reality. In particular, the Tennessee Eastman (TE) challenge problem (Downs and Vogel, 1993) proved to be successful in this sense because of its plant-wide nature, its high nonlinearities, its constraints and its unknown model.

Despite the numerous studies performed on the TE problem, some observed behaviour remain difficult to understand because of the intrinsic complexity of the problem. This suggested the need for a medium-sized process where the multivariable and nonlinear context would be kept, while still being easy to decipher (Ricker, 1993).

This is the context that motivates the work of Ricker (1993), where a simplification of the TE is presented. The system proposed is a single unit that shows all the main characteristics of the original problem. Some work has been done on the application: traditional control strategies showed poor performance, while advanced techniques resulted in stability problems.

1.1 Objectives

The main goal of this work is to improve control performance and stability of the two-phase reactor presented in Ricker (1993). The main challenges posed by this application are the large nonlinearities and the constraints on both inputs and outputs.

Three control strategies will be compared. First a decentralized mixed strategy will be used in order to see the improvement given by the substitution of a PI controller with a monovariable MPC controller. Then, as suggested by the multivariable and constrained nature of the problem, a fully centralized MPC approach will be implemented on the system. Finally, because of the nonlinearities and the changing conditions the use of adaptation techniques will be explored.

Furthermore the possibility of using model adaptation techniques on a multivariable, highly nonlinear application was considered of particular interest.

1.2 Organization of the thesis

Chapter 2 points out the most important characteristics of the Tennessee Eastman problem and provides a detailed description of the two-phase reactor considered. Furthermore, the challenges posed by the problem are highlighted, some important considerations are pointed out and previous works are presented.

Chapter 3 is divided into three parts: first an overview on Model Predictive Control (MPC) is given, then a mixed strategy is tested and finally a multivariable MPC is introduced. For each strategy details are provided and relevant tuning parameters are discussed. Comparisons with the classical multiloop PI structure are shown and analyzed.

In Chapter 4 an attempt to efficiently deal with nonlinearities and changing conditions is presented. The approach chosen is Model Weighting Adaptation (MWA). First an overview of the algorithm is presented and then the extension to the multivariable case is shown. Both approaches of the algorithm are implemented and the resulting performance is discussed. Finally, the well known Recursive Least Square Adaptation is used to compare some of the results found with the MWA approach.

In Chapter 5 the main results of this work and the problems encountered are summarized. A series of recommendations and suggestions for future works are also discussed.

CHAPTER 2 Description of the problem

2.1 The Tennessee Eastman Challenge Problem

For many years the process control community has expressed interest in a benchmark simulation to test and compare different control strategies (Foss, 1973). In the years between 86 and 96 there has been some follow-up of this interest, such as the semi-batch reactor proposed by Chylla and Haase (1990), the fluidized catalytic cracker proposed by McFarlane *et al.* (1990) or the crude fractionator proposed by Shell (Prett and Morari, 86). In this sense Downs and Vogel gave their contribution and published the plant-wide Tennessee Eastman challenge problem, which will be referred to as TE from now on (Downs and Vogel, 1993).

The TE benchmark has some advantages compared to other problems of the same kind because it is a realistic problem, with the complexity and the challenges of an actual plant. In fact, Downs and Vogel took inspiration from an actual process that they encountered a few years before at the Eastman Chemical Company, and found it very suited as a test problem. To protect the proprietary nature of the real process, they changed the components, kinetics and operating conditions, while attempting to keep the behavior of the real process. In Downs and Vogel (1993) a qualitative description of the process is given, together with steady-state mass balance and a set of operating conditions and general objectives. A FORTRAN code has been made available to the scientific community, but Downs and Vogel decided not to publish the model equations, probably increasing the challenging aspect of the problem even more.

The process produces two products (G, H) from four reactants (A, C, D, E) according to the following equations:

$$A_{gas} + C_{gas} + D_{gas} \longrightarrow D_{liquid}$$
$$A_{gas} + C_{gas} + E_{gas} \longrightarrow H_{liquid}$$

An inert (B) is also present in the feeds and two side reactions give a by-product (F):

$$A_{gas} + E_{gas} \longrightarrow F_{liquid}$$
$$3D_{gas} \longrightarrow 2F_{liquid}$$

The reactions are highly exothermic and irreversible, and they take place in a two-phase, open-loop unstable reactor. Reactants are gaseous and non-condensible, while the products are liquid but slightly volatile. The reactions are catalyzed by a non-volatile liquid catalyst. There is no liquid stream leaving the reactor, so unreacted species and products leave the reactor in gas form, go through a partial condenser and then are treated in a liquid-vapor separator. The gas phase leaving the separator is recycled to the reactor feed and a purge is present in order to avoid inert and by-product build-up. The liquid phase goes through a reboiled stripper to purify the products.

The simulated plant has 12 manipulated variables and 41 measured outputs. The following figure presents the flowsheet of the process:

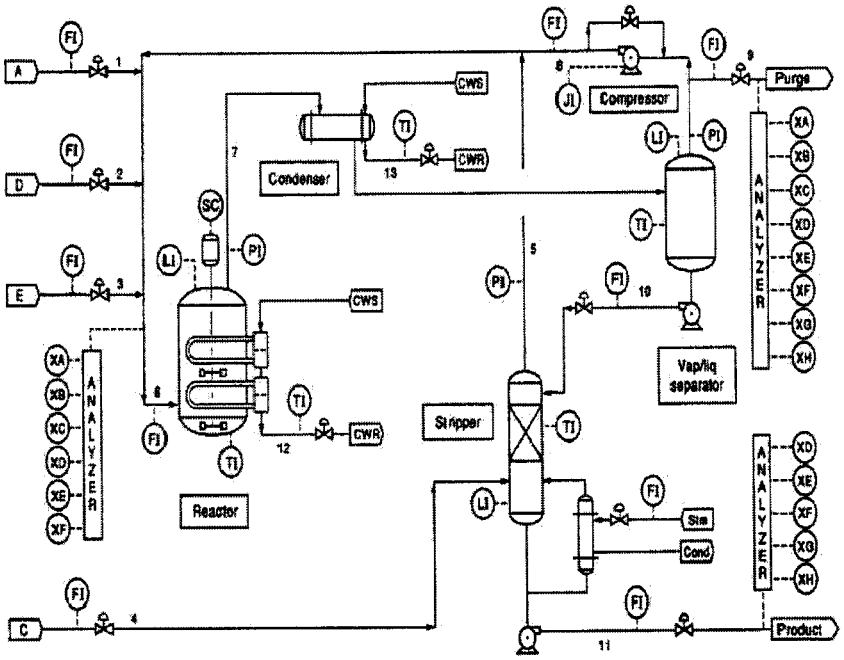

Figure 2.1: Flowsheet of the Tennessee Eastman process (taken from Downs & Vogel, 1993)

Since its publication, the TE has proven to be a success as a challenge problem for the process control community. Works range from classical multiloop PID approach (Ricker, 1996) to nonlinear model predictive control (Ricker and Lee, 1995) and from optimal steady-state operation (Ricker, 1995) to online optimization (Duval and Riggs, 2000).

Despite numerous works done on the subject, the TE challenge problem cannot be considered solved since a great margin for improvement is still possible.

2.2 The two-phase reactor as a simplification of the Tennessee Eastman

As shown before, the TE is a very interesting and challenging problem, but its complexity sometimes makes it difficult to understand certain behaviors of the process and of advanced control techniques, such as model predictive control.
With this motivation, Ricker (1993) simplificated the original problem. The goal was to have a process that would keep the same characteristics, the same behaviors and the same challenges of the TE, but that would be easier to understand and analyze.

The result is a single-vessel unit representing the reactor and the separation process of the Tennessee Eastman. This unit is a two-phase reactor (see Figure 2.2) where the following reaction takes place:

$$A_{gas} + C_{gas} \longrightarrow D_{liquid}$$

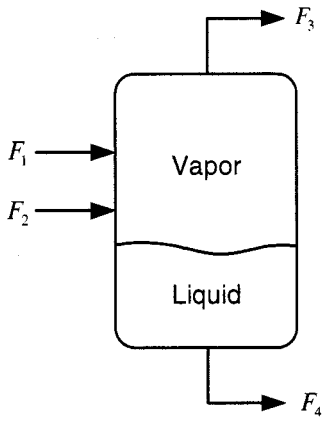

Figure 2.2: Scheme of the two-phase reactor

Reactants A and C are fed through the main feed (F_1), which contains impurities of an inert B. Another stream of pure A is available (F_2) in order to correct the A/C ratio. Reactants are gases and non-condensible, while product D is liquid and non-volatile. The reaction is catalyzed by a solid catalyst in the liquid phase, which implies that the reaction takes place at the liquid-vapor surface. Note that in Ricker (1993) there is no mention on the properties of D, so it is reasonable to assume that product quality is constant.

A purge flow (F_3) avoids inert and excess-reactant build-up in the reactor; F_3 depends on the reactor pressure and on the valve opening. Pure D is removed from the bottom of the reactor through a fourth stream (F_4); this stream is manipulated by a built-in proportional (P) controller on the liquid inventory (*liq*) whose setpoint is available for manipulation and represents one of the manipulated variables of the system. This makes the reactor open-loop stable.

Measured outputs include flow measurements, pressure, liquid inventory, and chemical composition of the purge flow. The composition measurements are available with a sampling time of and a delay, both of 6 minutes. The manipulated variables are the valve openings for streams F_1, F_2 and F_3 and the liquid inventory setpoint.

Operating constraints are present on the reactor pressure, which cannot exceed 3000 kPa (shut-down limit) and on the liquid inventory, which has to be kept between 0% and 100%. For obvious reasons, constraints on valves (0-100%) are also present. It will be shown further that the constrained character of this system is a very important aspect of the problem, and the design of control strategies must account for this.

Despite all the simplifications, it can easily be shown how close this system is to the original TE problem: the organization of the feeds, the presence of an inert and the consequential need for a purge, the operating and input constraints and the composition

measurements dynamics are just a few examples. It could also be shown that the two systems not only are similar from a physical point of view, but also that they present the same characteristic dynamic behaviors, such as nonlinearities and gain sign inversions.

The similarities suggest that valuable results found for the simplified system – or the understanding obtained from these results – could be applied to the more complex TE.

Nevertheless, it is important to point out some differences:

- in the original TE process the temperature dynamics are considered because of the highly exothermic reactions taking place in the reactor; in the two-phase reactor presented in Ricker (1993) an isothermal behavior is assumed
- the original TE problem presents a recycle stream that complicates the dynamics and the control of the system; in the two-phase reactor this aspect is not considered

2.2.1 Dynamic Model

Molar balances on the different species give the following differential equations:

$$\frac{dN_A}{dt} = y_{A1}F_1 + F_2 - y_{A3}F_3 - R_D \qquad [kmol\ h^{-1}] \qquad (2.1)$$

$$\frac{dN_B}{dt} = y_{B1}F_1 - y_{B3}F_3 \qquad [kmol\ h^{-1}] \qquad (2.2)$$

$$\frac{dN_C}{dt} = y_{C1}F_1 - y_{C3}F_3 - R_D \qquad [kmol\ h^{-1}] \qquad (2.3)$$

$$\frac{dN_D}{dt} = R_D \qquad [kmol\ h^{-1}] \qquad (2.4)$$

where:

- N_i represents the number of moles of species i
- y_{ij} represents the mole fraction of species i in stream j
- F_j represents the stream j in terms of $kmol\ h^{-1}$
- R_D is the reaction rate ($kmol\ h^{-1}$)

The reaction rate is given by the following equation:

$$R_D = k_0 P_A^{1.2} P_C^{0.4} \qquad [kmol\ h^{-1}] \qquad (2.5)$$

where k_0 is a pseudo-reaction constant which takes into account kinetics (activation energy), external diffusion (between the gas and the liquid) and internal diffusion (in the solid catalyst suspended in the liquid phase). It is important to remember that it is assumed that the reactor operates isothermally and at conditions such that the pseudo-reaction constant doesn't change (constant impeller speed, constant gas-liquid contact area, etc.).

Furthermore P_i, the partial pressure for species i, is given by:

$$P_i = P y_{i3} \qquad [kPa] \qquad (2.6)$$

where P follows the ideal gas law:

$$P = \frac{(N_A + N_B + N_C) \cdot R \cdot T}{V_V} \qquad [kPa] \qquad (2.7)$$

with T=373K (assumed constant), R=8.314 ($kJ\ \ kmol^{-1}\ \ K^{-1}$) and V_V the total vapor volume in the reactor, which is given by

$$V_V = V_{TOT} - V_L \qquad [m^3] \qquad (2.8)$$

where:

$$V_{TOT} = 122m^3 \quad \text{and} \quad V_L = \frac{N_D}{\tilde{\rho}_L} \qquad [m^3] \qquad (2.9)$$

Note that liquid inventory measurement (*liq*) is expressed as a percentage of the maximum volume available for liquid:

$$liq = \frac{V_L}{V_{L\max}} \qquad (2.10)$$

As the gas phase of the reactor is assumed perfectly mixed, the composition in the purge flow is the same as in the reactor:

$$y_{i3} = \frac{N_i}{N_A + N_B + N_C} \qquad (2.11)$$

Feed flows 1 and 2 are linear functions of the valve opening:

$$F_i = F_{i,\max}\frac{\chi_i}{100} \qquad i = 1,2 \qquad [kmol\ h^{-1}] \qquad (2.12)$$

On the other hand, streams 3 and 4 are not only proportional to the valve opening, but they depend also on the pressure in the reactor. The resulting equation is:

$$F_i = \frac{\chi_i}{100} C_{v,i}\sqrt{P-100} \qquad i = 3,4 \qquad [kmol\ h^{-1}] \qquad (2.13)$$

All the valves follow first order dynamics on their command signals, which is user specified for valve 1, 2 (feeds) and 3 (purge), and dictated by the P controller on the liquid inventory for valve 4 (product flow).

$$\frac{d\chi_i}{dt} = \frac{1}{\tau_V}(u_i - \chi_i) \qquad i = 1,2,3 \qquad [s^{-1}] \qquad (2.14)$$

$$\frac{d\chi_4}{dt} = \frac{1}{\tau_V}[K_C(u_4 - liq) - (\chi_4 - \overline{\chi}_4)] \qquad [s^{-1}] \qquad (2.15)$$

Note that in equation 2.15 the command signal to the valve is given by the P controller on the liquid inventory (*liq*), and the term $\overline{\chi}_4$ is the steady-state opening of the valve at the nominal operating point

An instantaneous cost is also included to measure the operating cost per unit of component D produced.

$$C = \frac{F_3}{F_4}(2.206 y_{A3} + 6.177 y_{C3}) \qquad [\$\ kmol^{-1}] \qquad (2.16)$$

The following table summarizes the numeric values of all the constants stated above:

Table 2.1 : Numeric values of the constants of the two-phase reactor

Constant	Value and units
y_{A1}	48.5 %
y_{B1}	0.5 %
y_{C1}	51 %
k_0	$1.17 \times 10^{-3}\ kmol\, h^{-1}\ kPa^{-1.6}$
V_{TOT}	122 m^3
$V_{L\max}$	30 m^3
$\tilde{\rho}_L$	8.3 $kmol\ m^{-3}$
$F_{1,\max}$	330.46 $kmol\ h^{-1}$
$F_{2,\max}$	22.46 $kmol\ h^{-1}$
C_{v3}	0.00352
C_{v4}	0.0417
τ_V	10 s
$\overline{\chi}$	47.03
K_C	-1.4

The resulting model has 8 states, 10 outputs and 4 manipulated variables which are summarized in the following tables:

Table 2.2 : States of the two-phase reactor

State variable	Nominal value	Description	Symbol	Units
x_1	44.5	Molar holdup of A	N_A	*kmol*
x_2	13.5	Molar holdup of B	N_B	*kmol*
x_3	36.6	Molar holdup of C	N_C	*kmol*
x_4	110.0	Molar holdup of D	N_D	*kmol*
x_5	60.9	Feed 1 valve position	χ_1	%
x_6	25.0	Feed 1 valve position	χ_2	%
x_7	39.3	Purge valve position	χ_3	%
x_8	47.0	Product valve position	χ_4	%

Table 2.3 : Input variables for the two-phase reactor

Manipulated variable	Nominal value	Purpose	Range
u_1	60.9	Changes χ_1	0-100%
u_2	25.0	Changes χ_2	0-100%
u_3	39.3	Changes χ_3	0-100%
u_4	44.2	Setpoint for y_6	0-100%

Table 2.4 : Output variables for the two-phase reactor

Output variable	Nominal value	Description	Symbol	Units	Range
y_1	201.4	Feed flow 1 measurement	F_1	$kmol\ h^{-1}$	0-330.46
y_2	5.6	Feed flow 2 measurement	F_2	$kmol\ h^{-1}$	0-22.46
y_3	7.0	Purge flow measurement	F_3	$kmol\ h^{-1}$	See eq.
y_4	100.0	Product flow measurement	F_4	$kmol\ h^{-1}$	See eq.
y_5	2700.0	Pressure	P	kPa	<3000
y_6	44.2	Liquid inventory	liq[1]	% of max	0-100
y_7	47.0	A mole fraction in purge	y_{A3}	mol %	0-100
y_8	14.3	B mole fraction in purge	y_{B3}	mol %	0-100
y_9	38.7	C mole fraction in purge	y_{C3}	mol %	0-100
y_{10}	0.2415	Instantaneous cost	C	$\$\ kmol^{-1}$	> 0

2.2.2 The scenarios

Together with the complete model, some scenarios are provided to test the performance and the robustness of the different control strategies. These scenarios are meant to mimic the challenges given by disturbances and setpoint changes proposed in the original Tennessee Eastman challenge problem. Here follows a brief description of the different scenarios:

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[1] Note that the name of this variable has been changed from Ricker (1993) because the notation used there was not very clear with respect to the difference between liquid inventory (%) and liquid volume (m^3).

1. *Regulation during a disturbance in feed composition*: y_{A1} decreases step-wise from 48.5% to 45%, y_{C1} increases from 51% to 54.5%, while the inert content remains constant.

   The goal is to keep production rate within ± 5% of the nominal value; obviously, all the constraints on pressure and liquid inventory have to be satisfied at all time.

2. *Production rate increase*: production rate goes from 100 to 130 $kmol\ h^{-1}$ as quickly as possible.

   Note that in order to do that, steady state considerations on the reactor imply that pressure and y_{A3} have to be increased as well. The new setpoint for pressure is chosen at 2850 kPa and for purge flow composition at $y_{A3sp} = 63\%$.

3. *Sudden loss of Feed 2*. In case that pure A is no longer available (valve sticking, loss of holdup,...) the reactor has to work with an excess of C, which causes a decrease in production. The goal is to keep production as high as possible if the nominal value is not feasible.

4. *Drift in kinetic parameters*. Reaction constant k_0 shifts linearly over a 48 hour period from the nominal value of 1.17×10^{-3} to 1.10×10^{-3} while the exponent for P_c in the reaction rate law shifts from 0.4 to 0.35 over the same period of time.

5. *Change in purge concentration*. A setpoint change on y_{A3} from 47% to 63% is required. This could be done in order to reduce operating costs.

6. *Increase in inert content of Feed 1*. Stepwise increase of y_{B1} from 0.5% to 1%, y_{C1} decreases from 51% to 50.5%, while y_{A1} remains constant at 48.5%.

It must be recognized that the major challenge in this problem is disturbance rejection. In fact setpoint changes (scenarios 2 and 5) are considered relatively easy to implement with decent performance: response can be slow and sluggish but it is generally difficult

to violate constraints on pressure and liquid inventory. On the contrary, handling disturbances can be problematic. If a control structure is not accurately chosen, stability issues may arise and constraint violation can be an issue.

It is important to point out which, among the scenarios proposed in Ricker (1993), must be considered as the most difficult. Scenarios 1 and 3 are particularly problematic because they affect the system in a step-wise fashion that causes a relatively fast deviation from nominal operating point. Furthermore, if no control action is taken, these scenarios lead to constraint violation for pressure.
On the other hand scenario 4 takes place over a large amount of time (48 hours), nevertheless it must be considered as challenging due to the important change of operating conditions and the resulting unfeasibility of the nominal setpoint. The latter aspect is not particularly problematic if a multiloop strategy is used, but in the case of centralized MPC strategy may lead to stability problems.
In conclusion, for different reasons scenarios 1, 3 and 4 are the most challenging scenarios among the six proposed.

As previously mentioned, some scenarios lead to an unfeasibility of the nominal operating point. In this case offsets from setpoints are present at the final steady state. A good control structure will try to minimize the offsets according to priority of the variables. From a process point of view, production has to be maximized and purge chemical composition can be relatively important as well, depending on economic considerations. On the other hand, pressure and inventory deviation from the setpoint can be tolerated, under the condition that constraints are satisfied at all time and a certain safety margin is maintained.

2.2.3 Choice of the MVs and the CVs

In order to design a control structure of the process it is necessary to choose what outputs are going to be controlled, i.e. what the controlled variables (CVs) are going to be.

Possible candidates for the CVs are:

- F_1, F_2, F_3 or F_4
- Pressure (P)
- Liquid inventory (liq)
- Purge composition (y_{A3}, y_{B3} or y_{C3})
- Instantaneous cost (C)

Among the 10 outputs, there are some that are not interesting from a process control point of view, such as F_1, F_2 and F_3. On the other hand, P and liq have to be controlled since they are constrained outputs and failure to keep them within their normal ranges can result in an unexpected shutdown or improper operation of the unit.
Another key variable is F_4, which represents the product flow (stream 4). In order to have good reactor performance it is desirable to keep F_4 as high as possible and to reduce oscillations. This also has a positive effect on downstream units.
The fourth controlled variable could be either one of the composition in the purge flow (y_{A3}, y_{B3} or y_{C3}) or the instantaneous cost.
The instantaneous cost is a complex function of the system state and it is not easily correlated to the system performance. Furthermore it changes dramatically during transient conditions and it can correspond to different steady-states.

On the other hand, choosing one 'composition variable' as the fourth CV has some advantages. First, there is a unique steady-state operating point for the reactor corresponding to given values of the setpoints; second, economic considerations may

require that the amount of unused reactants leaving from the purge is tracked (one may want to increase the amount of B and decrease C as much as possible). However, this choice has a major drawback: for a given production rate and pressure, the feasible setpoint range for chemical composition is limited and dependent on the operating conditions.

It is important to note that there is a very close relationship between y_{A3}, y_{B3} and y_{C3} given by the steady state equations of the system. In fact, for a given pressure and production rate, fixing y_{A3} implies a precise value for y_{C3} (remember that at steady-state $F_4 = R_D = k_0 P_A^{1.2} P_C^{0.4}$) and y_{B3} can be calculated by the relationship $y_{B3} = 1 - y_{A3} - y_{C3}$. A similar reasoning is valid if we fix y_{B3} or y_{C3}. In conclusion, the composition control for the purge flow can be achieved by setting anyone of the three mole fractions

Another option could be to control the ratio of some flows (such as F_3 / F_1), but this is not a better choice than purge composition, since fixing such a variable doesn't prevent the system output from fluctuating in an undesirable fashion. In particular there is no control on the chemical composition, and, as a consequence, a perturbation in the feed composition would result in a floating of the mole fractions of the different species.

These considerations suggest what we may choose as controlled outputs: the production rate (F_4), the pressure in the reactor (P), the liquid inventory (liq) and the chemical composition in the purge flow (in terms of y_{A3}, y_{B3} or y_{C3}). Controllability considerations will determine which mole fraction will be chosen.

2.2.4 Controllability analysis

A popular way to analyze the system interactions and consequently the controllability is to examine the relative gain array (RGA) matrix. This methodology was first proposed by Bristol (1966), and is quite simple to use, requiring information only about the static gains of the system.

The RGA matrix can be calculated according to the following term-by-term product:

$$\Lambda = K \otimes (K^{-1})^T \tag{2.17}$$

$$\Lambda = \begin{bmatrix} \lambda_{11} & \lambda_{12} & \dots & \lambda_{1n} \\ \lambda_{21} & \lambda_{22} & \dots & \lambda_{2n} \\ \dots & \dots & \dots & \dots \\ \lambda_{n1} & \lambda_{n2} & \dots & \lambda_{nn} \end{bmatrix} \tag{2.18}$$

where K is the gain matrix of the system:

$$K = \begin{bmatrix} K_{11} & K_{12} & \dots & K_{1n} \\ K_{21} & K_{22} & \dots & K_{2n} \\ \dots & \dots & \dots & \dots \\ K_{n1} & K_{n2} & \dots & K_{nn} \end{bmatrix} \tag{2.19}$$

with K_{ij} gain of the i-th output over the j-th input

The RGA matrix is a measure of the interactions of the system, where each term represents the ratio between the open-loop gain and the gain with all of the other loops closed.

$$\lambda_{ij} = \frac{\left(\frac{\partial y_i}{\partial u_j}\right)_{open\ \ loop}}{\left(\frac{\partial y_i}{\partial u_j}\right)_{\substack{All\ \ loops\ \ closed \\ except\ \ u_j}}} \tag{2.20}$$

Ideally, a system with an RGA equal to the identity matrix (after column rearrangement) has no interactions at all, meaning that a change in each input will affect only one output at a time. From a control point of view, this means that the system can be viewed as n single-input single-output processes in parallel. More details on the RGA analysis can be found also in McAvoy (1984).

Also, an RGA matrix is very useful for choosing pairings in a multiloop approach. The elements closer to unity suggest the input and the output that should be paired. For a centralized strategy (such as multivariable Model Predictive Control) the RGA is nevertheless very useful. It provides an idea of the difficulty of the control problem since a 'uniform' RGA matrix (all elements close to each other) will imply a difficult control problem due to the interactions.

For obvious reasons, RGA analysis can be done on a specific set of manipulated and controlled variables. For the two-phase reactor presently considered, a final choice of controlled variables has not yet been made. Thus, different controllability analysis will be shown here, and the results will help to determine a final choice.

As stated previously concerning the relationship between the composition variables in the purge flow, we may choose one of the three mole fractions (y_{A3}, y_{B3} or y_{C3}) as a fourth controlled variable. Because of the presence of pure A feed (stream 2), y_{A3} is more attractive than y_{C3}; thus, the choice is between y_{A3} and y_{B3}.

In both cases the problem is simplified by the obvious choice of pairing the liquid inventory with u_4 (the inventory setpoint). This gives two alternative three-input, three-output systems.

'A' purge mole fraction is chosen as a controlled variable

In the first case the three outputs to be controlled are production rate (F_4), pressure (P) and purge composition in terms of A (y_{A3}). The gain matrix of this system is given in Ricker (1993) as following:

$$\Delta y = \begin{bmatrix} \Delta F_4 \\ \Delta P \\ \Delta y_{A3} \end{bmatrix} = K_1 \Delta u = \begin{bmatrix} 1.6208 & 0.1369 & -0.0835 \\ 46.5606 & -36.2879 & -9.1453 \\ -0.6766 & 1.5728 & 0.0711 \end{bmatrix} \Delta u \qquad (2.21)$$

And the corresponding Λ is:

$$\Lambda_1 = K_1 \otimes (K_1^{-1})^T = \begin{bmatrix} 1.24 & 0.03 & -0.26 \\ -0.43 & -0.14 & 1.56 \\ 0.19 & 1.11 & -0.30 \end{bmatrix} \qquad (2.22)$$

which suggest the following pairings:

- u_1 to control F_4
- u_2 t control y_{A3}
- u_3 to control P

'B' purge mole fraction is chosen as a controlled variable

The second option was to choose the B mole fraction in the purge flow as a controlled output, instead of y_{A3}. This yields the following gain matrix around the base case operating point:

$$\Delta y = \begin{bmatrix} \Delta F_4 \\ \Delta P \\ \Delta y_{B3} \end{bmatrix} = K_2 \Delta u = \begin{bmatrix} 1.6208 & 0.1369 & -0.0835 \\ 46.5606 & -36.2879 & -9.1453 \\ -0.12065 & 0.0997 & -0.3389 \end{bmatrix} \Delta u \qquad (2.23)$$

And the corresponding Λ is:

$$\Lambda_2 = K_2 \otimes (K_2^{-1})^T = \begin{bmatrix} 0.942 & 0.089 & -0.031 \\ 0.078 & 0.863 & 0.059 \\ -0.020 & 0.048 & 0.972 \end{bmatrix} \qquad (2.24)$$

The pairings suggested by this new choice of the MVs, suggests the following pairings:

- u_1 to control F_4
- u_2 to control P
- u_3 to control y_{B3}

At first glance, the second RGA seems better, since the elements corresponding to the pairings are closer to unity than they are in the first RGA. This means fewer interactions and therefore an easier system to control.

This consideration may lead us to choose the second control structure instead of the first one. But this choice is falsely appealing because pressure control suffers from a serious problem: the gain sign inversion presented by the controlled system.
Controlling the pressure with Feed 2 (pure A) exploits a transfer function with gain sign inversion at certain conditions. For example, if the system is poor in A, an increase in Feed 2 will cause a decrease in pressure, but if the system is rich in A (high y_{A3}), an increase in Feed 2 will cause an increase in pressure. We have to remember that the

reaction kinetic is bimolecular, and so a certain ratio between the partial pressures must be guaranteed in order to have high production.

The first control structure has some drawbacks as well, especially problems on control authority on P. In many conditions the purge valve (u_3) is likely to saturate and pressure control will have to rely on the movement of other manipulated variables, if possible. Of course, in the case of a multiloop strategy this is not possible and in such conditions pressure will be out of control unless an override structure is added. For a centralized approach this is less of a problem, but these considerations still lead to the conclusion that valve saturation will be an issue.

The main advantage of this structure is that the pairings suggested by the RGA do not present any gain sign inversion. This could be shown by analyzing the gain matrix (K) at different operating points, or more simply by physical observations:

- an increase in Feed 1 will always increase the production rate: if reactants are added at a faster rate, D will be produced at a faster rate as well
- opening the purge valve will always decrease the pressure (unless saturation problems are encountered)
- an increase in Feed 2 (pure A) will always increase the mole fraction of A in the gas phase

Considering what has been discussed so far, the first set of controlled variables will be chosen and will be used for the rest of this work. Furthermore this was the choice made in Ricker (1993), and having the same set of controlled outputs will give a more consistent basis for comparison.

2.3 Control strategies proposed by Ricker (1993)

The strategies discussed in Ricker (1993) are presented briefly. First a multiloop PI structure is implemented with a certain degree of success. Then a centralized linear MPC controller is designed to handle the 4×4 system (i.e. the liquid inventory setpoint is actually used). This structure gives acceptable performance for low demanding scenarios whereas performance is unacceptable in high demanding scenarios. In order to fix some of the problems encountered with the previous MPC controller, a decentralized approach is attempted; this approach works for all scenarios with a performance that can be considered comparable or better than the multiloop strategy.

2.3.1 Multiloop strategy

The first attempt is the most straightforward: controlling the system with a standard multiloop approach. The pairings follow the considerations on the RGA matrix and they are as follows:

- u_1 controls production rate (F_4)
- u_2 controls composition in terms of A (y_{A3})
- u_3 controls reactor pressure (P)

As mentioned above, the main problem with this structure is given by control authority for the pressure loop: when valve 3 is saturated, pressure control is lost.
This suggests the need to use an override to prevent such a possibility. The override is added as a fourth feedback loop, measuring the pressure and manipulating the additional variable F_{4SP}^{adj}, which is a correction on the production rate setpoint; for obvious reasons, F_{4SP}^{adj} is equal or lower than zero.

The loops are regulated by discrete PI controllers expressed by the following velocity form:

$$\Delta u_n = u_n - u_{n-1} = K_c\left[e_n - e_{n-1} + \frac{\Delta t}{\tau_I} e_n\right] \tag{2.25}$$

Δt was chosen equal to 0.1, and the tuning parameters are given in the following table.

Table 2.5: Tuning parameters for multiloop strategy

Loop	K_c	τ_I (hours)
1	0.1	1.0
2	-0.25	1.5
3	2	3.0
4	0.7	3.0

2.3.2 Centralized linear Model Predictive Control

In an attempt to increase performance, a centralized form of linear Model Predictive Control (MPC) was used. In this case, the model used was a 4×4 and all the interactions were taken into account. MPC is well known for its ability to handle constraints and multi-input multi-output (MIMO) systems, so this seems a very sensible choice for this kind of problem. An overview of MPC will be discussed in section 3.1.

It is important to note that the 4×4 structure derives from the inclusion of the liquid inventory setpoint among the manipulated variables, whereas for the preceding approach it was kept constant at its nominal value. This change is due to the fact that

with a centralized strategy, liquid inventory fluctuations can be, at least in theory, used to compensate for temporary production rate variations.

The MPC used is in its standard quadratic form and it is based on a discrete, linear, time-invariant state-space model in the form:

$$\begin{aligned} x_{k+1} &= \Phi x_k + \Gamma u_k \\ y_k &= C x_k \end{aligned} \tag{2.26}$$

A state estimation strategy was included in order to handle unmeasured disturbance; the structure chosen is the standard Kalman filter (see Ricker (1993) for more details).

The penalty weights for manipulated and controlled variables are chosen according to the priority given to each controlled variable and the smoothness required to move each manipulated variable. Key considerations were:

- maximum production
- loose control for pressure and liquid inventory
- smooth variations of liquid inventory

The final values are:

$$\Lambda_y = diag\{3.0 \quad 0.1 \quad 1.0 \quad 0.1\}$$
$$\Lambda_u = 2 \cdot diag\{1.0 \quad 1.0 \quad 1.0 \quad 2.0\}$$

This approach works fairly well for minor disturbances and for minor setpoint changes, but not under the demanding conditions given by the previously described scenarios. Above all, stability problems are encountered at operating conditions far from the nominal case. Ricker identified the cause as the gain sign inversion of the P/u_2 transfer function. This was not an issue for the multiloop strategy since that transfer function is

off the main diagonal of the rearranged transfer function matrix, and it was considered a system interaction.

Moreover, stability problems occur when the system is close to hard constraints.

2.3.3 Decentralized linear Model Predictive Control

In order to correct the stability problems encountered with the previous approach, a decentralized strategy was tested.

The decentralized methodology is given by the fact that many of the transfer functions in the dynamic matrix are neglected (10 out of 16). In particular, troublesome or neglible transfer functions are simply set to zero. This solution certainly introduces some extra modeling error, but it has proven to be more robust than the centralized strategy.

A comparison between this approach and the multiloop strategy is not easy. Decentralized MPC definitely performs better for some scenarios, but it gives very different results for scenarios where persistent disturbances are involved. For example, for scenario 3 multiloop control gives a smooth decrease in production rate from the point where the disturbance appears. Alternatively, decentralized MPC keeps F_4 close to its nominal value and then lets it drop quickly as the liquid inventory approaches its lower bound. The choice of the appropriate approach will depend on considerations on the downstream units.

2.4 Concluding remarks

In this chapter the problem of the continuous two-phase reactor developed by Ricker (1993) was presented. It is a simplification of the Tennessee Eastman process which keeps all the main behaviors and challenges of the original problem.

The details of the model were presented and some basic studies have been carried out, such as the choice of the controlled variables and controllability analysis (RGA). The most important characteristics have been identified in nonlinearities (notably in the form of gain sign inversion) and in the constrained nature of the inputs and of some of the outputs.

This was particularly evident analyzing the previous works done on the same application. Stability problems occured with a centralized MPC approach, and a multiloop PI control showed poor performance. A decentralized MPC didn't present stability problems but its performance is not clearly better than the multiloop approach.

CHAPTER 3 Model Predictive Control

In this chapter an overview on MPC is presented and then two different strategies for the problem considered will be developed. The first approach is a multiloop mixed strategy presenting both PI controllers and MPC. The second approach is based on a fully centralized MPC controller.

3.1 Overview on Model Predictive Control

Model Predictive Control (MPC) is the class of advanced process control technique most widely used in the industry with thousands of successful applications. The reasons for this success reside in its ability to handle constrained systems (input and output) and its simplicity in treating multivariable systems. Moreover, MPC is a model-based technique and it gives an near-optimal control (Bequette, 2003).

Even if the class of Model Predictive Control algorithms includes many different formulations, the following three aspects can be identified:

-it is a model-based technique

-it gives an 'optimal' solution

-it uses a receding horizon approach

3.1.1 Model

One of the key characteristic of MPC is that it incorporates a model of the process. The model used can be either linear or non-linear. If a nonlinear model is used, we speak of nonlinear MPC (NMPC); this approach is not going to be discussed here since it is outside the scope of this thesis but a good survey can be found in Mayne *et al.* (2000).

In the case of linear model, three different types of model are possible: transfer function, state-space representation or step response model.

Transfer function

The first form uses the formulation typical of the adaptive control area and it is used in the context of General Predictive Control (GPC, see Clarke (1987) for more details). In this case the model is expressed as:

$$A(q^{-1})y(t) = B(q^{-1})u(t-1) \tag{3.1}$$

where A and B are polynomials in the backward shift operator q^{-1} (the details of this notation will be clarified in section 4.2.1).
This approach is less widely used than the two others.

State-space representation

The second form is given by a classical discrete-time state-space representation in the form given in Rawlings (2000) or in Maciejowski (2002):

$$\begin{aligned} x_{k+1} &= \Phi x_k + \Gamma u_k \\ y_k &= C x_k \end{aligned} \tag{3.2}$$

This approach is computationally more attractive and theoretically elegant .

Step response

The use of the step response model is the more traditional approach and also the more intuitive one. In this case the system is represented by:

$$\hat{y}_k = \sum_{i=1}^{N-1} s_i \Delta u_{k-i} + s_N u_{k-N} \qquad (3.3)$$

The notation used follows the explanation given in Bequette (1993) and partly in Ogunnaike (1994) and it is as follows:

- $\hat{y}_k$ is the predicted output at time k
- N is the model length
- u_{k-N} is the system input at time k-N
- Δu_{k-i} is the incremental input at time k-i
- $[s_1, s_2, ...s_N]$ are the coefficients of the step response, that is:

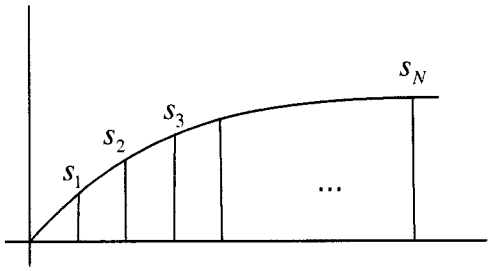

Figure 3.1 : Step response model

The main drawback of this approach is that it leads to more demanding computations. Nevertheless, one major advantage is evident: no special identification procedure is needed, since input-output data from a step test is sufficient. Another advantage is that many available MPC algorithms (such as Matlab/Simulink MPC Toolbox) are based on

this representation. Additionally, this approach is more logical when output-feedback control is used, rather than state-feedback.
Because of its simplicity and intuitiveness the step response model will be used in this thesis.

Note that MPC is inherently a discrete-time algorithm, so models for the system have to be in discrete forms.

3.1.2 Optimality

MPC optimality derives from the fact that control actions are calculated as the result of the optimization of a performance objective. A performance measure includes the predicted output deviations from a given reference trajectory and penalties on excessive control moves (even though this is omitted in some formulations). Output error can be expressed in term of absolute value or quadratic error, but the latter option is more common because of its computational implication (Maciejowski, 2002). Control move penalty is generally expressed in the same form as output error.
Outputs are predicted over a prediction horizon P, and they are calculated by applying a given input trajectory to the known model. The calculated control moves are over a control horizon M and they represent the optimization independent variable.

Concerning optimality, it is important to point out that MPC can be derived from optimal control theory. MPC is essentially a finite-horizon discrete-time optimal controller and this yields a sub-optimal solution to the infinite horizon problem. More details on suboptimality can be found in Primbs (1993).

The use of quadratic error and input penalty leads to the Quadratic Dynamic Matrix Control formulation (QDMC). This formulation, together with a linear process model

leads to a quadratic program (QP) optimization, for which many algorithms exist (Rawlings, 2000).

For the SISO case, the described optimization at time k is expressed mathematically by the following equation:

$$\min_{\Delta u_k,\ldots,\Delta u_{k+M-1}} \left[\sum_{i=1}^{P} (r_{k+i} - \hat{y}_{k+i})^2 + w \sum_{i=0}^{M-1} \Delta u_{k+i}^2 \right] \tag{3.4}$$

where

- r_{k+i} is the reference trajectory (setpoint) at sampling k+i
- $\hat{y}_{k+i}$ is the predicted output at sampling k+i
- Δu_{k+i} is the incremental control action at sampling k+i
- M is the control horizon
- P is the prediction action
- w is the relative weight for control action

For the MIMO case, in order to assign priorities to the different inputs and outputs, different weighting factors are assigned to each variable. The formulation obtained is very similar, but matrices and vectors replace the scalars. See Ogunnaike (1994) for more details.

Note that if the step-response representation is used, at time *k* system output can be easily predicted by the following formula (details in Bequette, 2002):

$$\underline{\hat{y}} = \underbrace{\begin{bmatrix} \hat{y}_{k+1} \\ \hat{y}_{k+2} \\ \vdots \\ \hat{y}_{k+j} \\ \vdots \\ \hat{y}_{k+P} \end{bmatrix}}_{P\times 1} = \underbrace{\begin{bmatrix} s_1 & 0 & 0 & \cdots & 0 \\ s_2 & s_1 & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & & \vdots \\ s_j & s_{j-1} & s_{j-2} & \cdots & s_{j-M+1} \\ \vdots & \vdots & \vdots & & \vdots \\ s_P & s_{P-1} & s_{P-2} & \cdots & s_{P-M+1} \end{bmatrix}}_{P\times M} \underbrace{\begin{bmatrix} \Delta u_k \\ \Delta u_{k+2} \\ \vdots \\ \Delta u_{k+M-1} \end{bmatrix}}_{M\times 1} + \underline{\hat{y}}^F = S_f \underline{\Delta u} + \underline{\hat{y}}^F \quad (3.5)$$

where $\underline{\hat{y}}^F$ represents the effect of past control moves ('free response' of the system) and S_f is called dynamic matrix. Note that that the approach described here is also called Dynamic Matrix Control (DMC). Details can be found in Cutler and Ramaker (1980).

For the MIMO case, this is extended to:

$$\underbrace{\begin{bmatrix} \underline{\hat{y}}_1 \\ \vdots \\ \underline{\hat{y}}_{ny} \end{bmatrix}}_{(P\cdot ny)\times 1} = \underbrace{\begin{bmatrix} S_{f\_1,1} & \cdots & S_{f\_1,nu} \\ \vdots & \ddots & \vdots \\ S_{f\_ny,1} & \cdots & S_{f\_ny,nu} \end{bmatrix}}_{(P\cdot ny)\times(M\cdot nu)} \underbrace{\begin{bmatrix} \underline{\Delta u}_1 \\ \vdots \\ \underline{\Delta u}_{nu} \end{bmatrix}}_{(M\cdot nu)\times 1} + \underline{\hat{y}}^F = \underline{\underline{\beta}}\,\underline{\Delta u} + \underline{\hat{y}}^F \quad (3.6)$$

where $\underline{\underline{\beta}}$ is the dynamic matrix for the MIMO system, *ny* is the number of controlled variables, *nu* is the number of manipulated variables and $\underline{\hat{y}}^F$ represents the 'free response' of the MIMO system. Further details can be found in Ogunnaike (1994).

3.1.3 Receding horizon

In order to guarantee accurate tracking of the reference trajectory, MPC is implemented in a receding horizon fashion (MPC is also called Receding Horizon Control (RHC) or Moving Horizon Control (MHC)).

This means that at each sampling time actual outputs are measured and the error between predicted and measured values is used to compute another open-loop optimization. This implies that at each sampling time the optimization has to be computed again and that only the first control action is actually applied to the plant.

For the DMC algorithm used in the work of this thesis, prediction error is generally incorporated in the prediction using the assumption of the "constant additive disturbance", that is assuming that the present discrepancy between predicted and actual output will remain constant for the entire prediction horizon:

$$\hat{d}_{k+P} = \hat{d}_{k+P-1} = \ldots = \hat{d}_{k+1} = d_k = y_k - \hat{y}_k$$

Using the notation introduced earlier, the 'corrected' output prediction is calculated as follows:

$$\underline{\hat{y}} = S_f \underline{\Delta u} + \underline{\hat{y}}^F + \underline{\hat{d}}$$

It is important to note that more elaborate techniques exist in order to better estimate the effect of the term $\underline{\hat{d}}$. These imply the use of an observer and can improve the regulatory closed-loop performance of the MPC controller but, on the other hand they increase the number of tuning parameters. The design of an observer was not considered for the work of this thesis.

Note that the optimization performed is open-loop, and this receding horizon structure is the equivalent of adding feedback to the control system. Even in the unlikely case of a perfect model, this structure is justified by the need to reject disturbances.

This procedure can seem computationally very heavy, but it must also be considered that a closed-form solution is known for the unconstrained case and, if constraints are added, many very efficient QP algorithms are available. Nevertheless in some cases computational aspects can become an issue.

The MPC algorithm can be summarized in the following steps:

1. output measurements are taken
2. error on output predicted at last sampling time is computed
3. optimization is performed
4. first control action is implemented
5. the same procedure is repeated at next sampling time

The MPC structure can be viewed easily in the well known graph shown below.

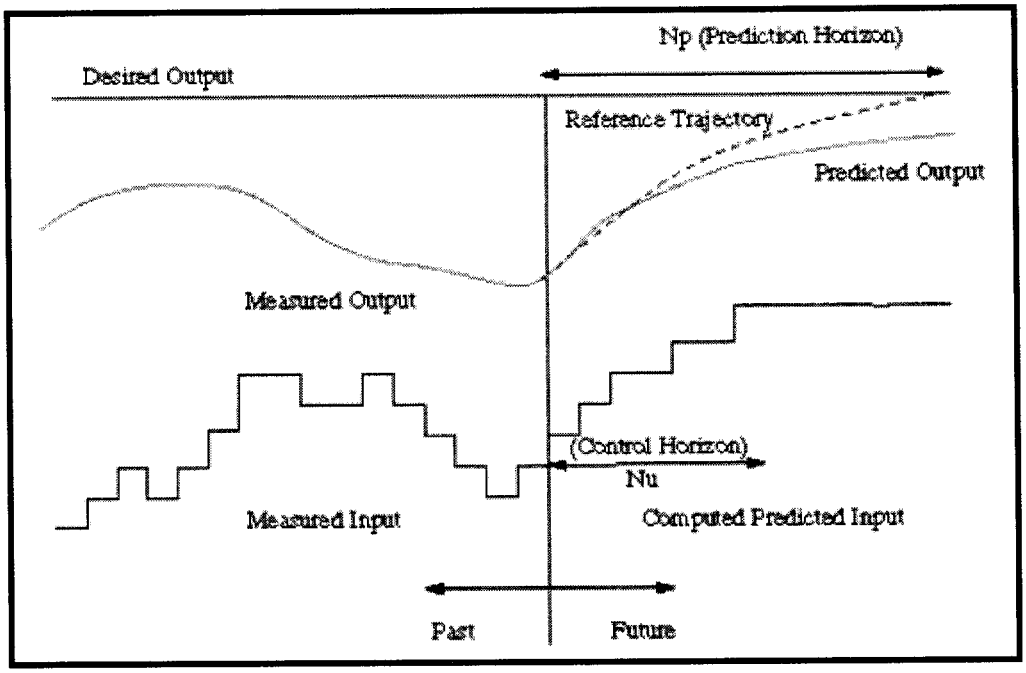

Figure 3.2: Basic concept of Model Predictive Control

As stated above, MPC is well suited to handle constraints. Constraints can be on manipulated and on controlled variables and they can be in terms of absolute value or in terms of variation rate. Constraints are generally expressed as:

$$y_{MIN} < \hat{y} < y_{MAX}$$

$$\Delta y_{MIN} < \Delta \hat{y} < \Delta y_{MAX}$$

$$u_{MIN} < u < u_{MAX}$$

$$\Delta u_{MIN} < \Delta u < \Delta u_{MAX}$$

These are easily included as constraints on the optimization algorithm.

3.2 Mixed strategy

3.2.1 Motivation

As seen in the previous chapter, the results found in Ricker (1993) show that for the two-phase reactor described a multiloop PI strategy has very poor performance and a centralized MPC shows serious robustness issues.

Within this chapter a mixed strategy will be attempted. The proposed approach is very similar to the multiloop PI approach, but with one of the loops controlled by a Single-Input Single-Output (SISO) MPC instead of a standard PI controller.

The objective is to observe the degree of improvement that can be achieved with a model based controller capable of dealing with input and output constraints. It will be shown that a certain degree of improvement is possible, but the major limitations given by the multiloop SISO approach remain.

3.2.2 Choice of the pairing for MPC

At this point it must be decided to which of the loops MPC approach will be applied. The following loops were suggested by the RGA analysis and used for multiloop PI strategy:

- u_1 to control F_4
- u_2 to control y_{A3}
- u_3 to control P

The following considerations will help us to understand which is the best choice.

MPC is very well suited for constrained (input and output) systems, so a sensible choice would be to apply it to the loop where this aspect is most important. Analyzing the results given by the multiloop strategy in Ricker (1993) (see Figure 3.4 to Figure 3.15), we see that in most scenarios manipulated variable u_3 hits either its upper or lower limits. This could also be expected from the control authority considerations done in chapter 2.

Moreover, pressure is a key variable because of its influence on the process and because it is the only constrained output, with a shutdown-limit at 3000 kPa [2].

One of the reasons for the poor performance given by the multiloop PI strategy was the excessive smoothness and slowness in control actions. Manipulated variable u_3 suffered particularly, since it must be moved more quickly and over a wider range than u_1 and u_2.

These considerations lead to the decision of implementing MPC on the pressure loop.

3.2.3 Identification of the model

In order to design a MPC, a model of the system to be controlled has to be obtained. Since a SISO approach is used, only a model of P/u_3 is necessary.

In this section, some general characteristics of the P/u_3 will be shown, and then a final choice of the model to be used will be presented.

A set of steps on u_3 of different amplitudes and signs have been applied to the open-loop system giving the following results:

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[2] Remembering that liquid inventory is handled by the built-in controller

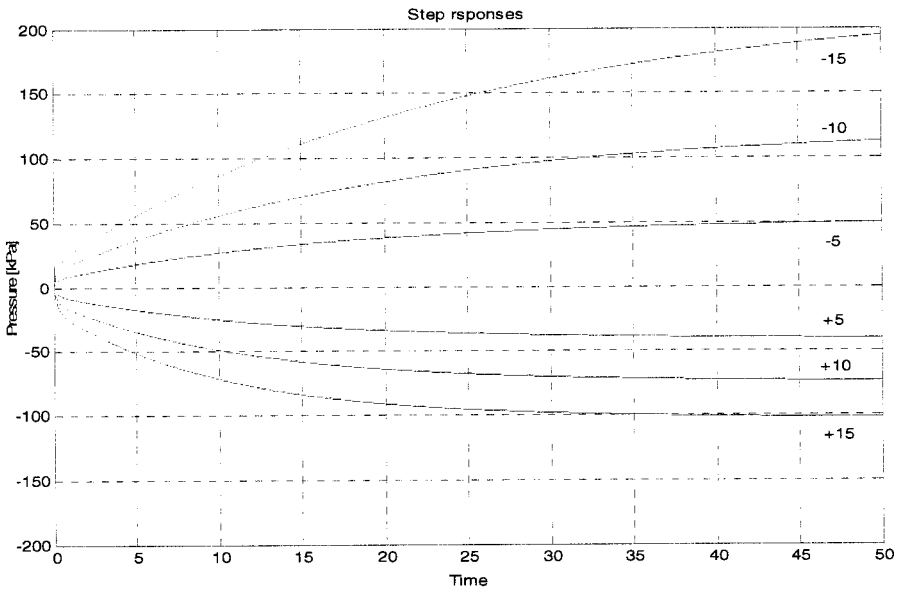

Figure 3.3 : Pressure responses to different step tests on u_3

It can be seen that the gains are dependent on the amplitude and on the sign of the step. This is an indication of the nonlinear behaviour of the system. It can also be observed that all the responses have a similar pattern:

- a *fast* component of the response (settling time between 1 and 3 hours): very similar for all the curves and almost proportional to the step amplitude
- a *slow* component of the response (settling time between 30 and over 50 hours): quite different for each curve in amplitude and in dynamics (a step of -15% has a much slower response than a +15% step)

The "*fast* component" can be explained as the *physical* response of the system: the reactor pressure changes because a higher opening of the purge valve gives a higher F_3. It is logical sense that this contribution is almost proportional to the step size (increase or decrease of the valve opening).

The "*slow* component" of the response is given by the *chemical* response of the system: as pressure drops or rises, operating conditions change and so does the chemical composition in the reactor gas-phase; this affects all the variables of the system in a nonlinear fashion, which explains the difference in settling times and final values.
Note that this pattern of response is encountered at all operating conditions (see fig A.1 in the Appendix).

These considerations lead to the conclusion that, in order to be representative of the system, a model for MPC, should present this particular pattern of response.

Before obtaining a 'final' model for the MPC, a choice on the type of representation (transfer function, state-space or step response) has to be made because this decision has some implications in the identification process. The step response model was chosen because of its simplicity and intuitiveness. Furthermore this allows the use of the Matlab/Simulink MPC Toolbox.

A model of the system could be obtained in different ways, but given the slow dynamics of the plant considered, more complicated identification signals such as PRBS were not considered because they would be potentially extremely time consuming (days or weeks). Furthermore, since step response model is used, a single step on the manipulated variable seems a more reasonable choice. Consequently, step amplitude and sign have to be chosen for the test.
Step amplitude has to be large enough to observe a 'realistic' response of the system (i.e. including part of the nonlinear dynamics); on the other hand, the system identification has to be done around a given operating point and a too large step size will show the system response over a range of operating points. The final choice will be a trade-off between these needs.

Another necessary choice is the sign of the step change; in this sense, the step with the higher gain was chosen in order to have an gain over-estimation of the system response for robustness reasons.

The final choice was for a step of - 5% which gave the response shown in Figure 3.3.

Since a step model is used for MPC, it is not strictly necessary to find a model fitting this curve and step response coefficients could be obtained from the actual plant output. Nevertheless, in order to have a simple representation of the model and in order to test system nonlinearities, a transfer function representing this data was found. This also allows for more flexibility in the simulation phase, where model length can be changed easily.

The continuous-time P/u_3 transfer function is in the following form:

$$g_{ID} = \frac{P}{u_3} = \frac{K(\xi s+1)}{(\tau_1 s+1)(\tau_2 s+1)} \tag{3.7}$$

with the following parameters:

Table 3.1 : Values of g_{ID} parameters

K	-10.42
ξ	2.2
τ_1	0.3
τ_2	16

The fit of the two graphs (identified transfer function and actual plant) is not shown here since they coincide perfectly.

3.2.4 Final structure

As explained before, the first attempt to improve control performance of the two-phase reactor was to replace one of the loops with a linear single-input single-output (SISO) MPC capable of handling constraints. The selected loop was the pressure loop, with purge valve as a manipulated variable.

It is important to point out that replacing a standard PI controller with an MPC for pressure loop, doesn't eliminate the control authority problems discussed in the previous chapter. This implies that an override structure has to be added as it was done for the multiloop PI strategy.

For the same considerations in Ricker (1993), the override is going to determine a correction on production rate setpoint (i.e. the same structure is kept). This choice also allows a clear comparison of the two strategies. For the same reason, tuning for the PI controllers and the override is consistent with Ricker (1993).

In conclusion the final structure is the following:

- F_4 controlled by u_1 (PI)
- P controlled by u_3 (MPC)
- y_{A3} controlled by u_2 (PI)
- P (override) controlled by F_{4SP}^{adj} (saturated PI)

3.2.5 Tuning parameters

In this section the focus is on how to tune the MPC controller. Some general considerations are presented with particular focus on concerns related to the application under study.

As explained before, at each sampling time MPC control moves are calculated as the result of an open-loop optimization on the system. Tuning this kind of controller corresponds to choosing the parameters of the optimization, which, for the SISO case, are:

- T, sampling time for MPC
- N, model length
- P, prediction horizon
- M, control horizon
- w, control action weighting

Tuning of MPC controllers is always a delicate and sometimes troublesome procedure, for which some general guidelines are known, but no systematic procedure is effective for all situations. For the SISO case, this is generally not as problematic, but even for a small multivariable MPC controller, tuning can easily become very difficult and time consuming.

Sampling time and model length

The most straightforward parameters to choose are model length and sampling time. These two quantities are strictly related to each other: a smaller sampling time requires a longer model length (which is expressed as a number of sampling times). It is clear that, in order to have good prediction, the model should represent most of the actual system response (generally at least 90% of the final gain). Once the sampling time is chosen, the model length can be easily adjusted.

In order to choose sampling time, two factors need to be considered:

- smaller sampling times give tighter control and better disturbance rejection since they allow a better model of the process
- smaller sampling times lead to more heavy computation

It is important to consider that between two samples the system is open-loop, which means that during that time disturbances affect the system freely and any error on the system prediction is unmonitored. This suggests that high sampling times lead to a loose control and possibly to stability problems. As a rule of the thumb, reasonable sampling times are from one fourth to one tenth of the desired closed-loop time constant (Astrom and Wittenmark, 1984).

A final choice of T =0.1 hours was made with for the following reasons:

- this is consistent with the sampling time of the PI controller
- foreseeing an extension to the MIMO case, this choice is consistent with the sampled nature of the composition measurements
- it represents a good trade-off between performance and computational effort.

In order to have most of the plant response represented by the discrete model, a model length of 400 sampling times was chosen (corresponding to 40 hours) which guarantees an error on the final gain of only 8%.

Prediction and Control Horizon

Prediction horizon (P) is an important parameter for MPC controllers since it affects the length of prediction. P has to be chosen long enough so that the main trend of the system dynamics is considered. For example systems with an inverse response impose a P so that the final gain of the process is represented. In our case an excessively low P would lead to a prediction taking into account only of the fast dynamics. On the other hand high prediction horizons can pose computational problems.

Furthermore, P is known to have a stabilizing effect on the closed-loop system and it is generally assumed that a sufficiently long prediction horizon will stabilize the system. In the case of constrained systems this might not be true, as shown in Zafiriou (1991).

Control horizon is another key parameter to choose since it affects the aggressiveness of the controller. High control horizons generally give an aggressive and more performing control, while a low value for M is generally considered a 'safe' choice. In particular, for the choice of M=1 and P≥N, MPC moves the input in a steady-state fashion (i.e. giving an open-loop dynamics). For constrained problems this stabilizing effect of low control horizons doesn't necessarily hold (Zafiriou 1991).

Control action weighting

Control action weighting (w) is generally not a critical parameter to choose. Its goal is to limit excessively aggressive control actions and thus to avoid chattering of the manipulated variable. If prediction horizon P is much greater than control horizon M, w has no particular effect since in the optimization the contribution given by the output error is already much more important than the one given by control actions. In these cases, w can even be set to zero (Bequette, 1993).

In conclusion, the following parameters for MPC were chosen:

Table 3.2: Tuning for the linear SISO MPC of the mixed strategy

T	0.1 hr
N	400
P	60
M	10
w	1

3.2.6 Results for the mixed strategy

The control strategy described above was tested on a Matlab/Simulink simulation of the two-phase reactor under study. In the following figures, the results given by the multiloop PI strategy and by the mixed strategy are shown. Manipulated variables are also presented in order to observe control aggressiveness and to check for valve saturation phenomena.

It is important to point out that liquid inventory in this case is not a critical variable, since it is regulated by the built-in P controller. Nevertheless, trajectories of this variable are shown for coherence with the figures for the multivariable case.

In the case of a disturbance in Feed 1 composition (scenario 1) the main problem is a quick increase in pressure; additionally, y_{A3} drops and production rate is affected. Both control structures open the purge valve to accomodate the increase in pressure, but this is not sufficient and valve saturation is quickly reached. The override control reduces the production rate since t=0, because of the quick increase in pressure; Feed 2 is increased to compensate the deficit of A in the gas phase.

The main difference between these control strategies is that when pressure returns close to 2700 kPa, the MPC quickly desaturates the purge valve and consequently is capable of keeping pressure around its setpoint. This is clearly a due to the process model dynamics incorporated in the controller.

Production rate and purge composition are not affected by the change in the pressure trajectory. This is due to the relatively small interactions of the system suggested by the RGA matrix.

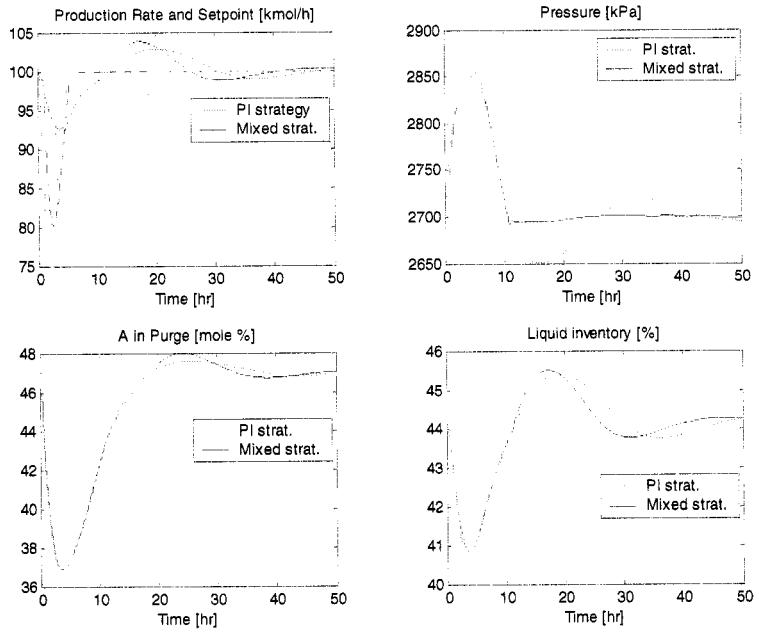

Figure 3.4: Scenario 1 – Controlled variables – PI strategy (green) and mixed strategy (black); production setpoint follows the same colours in a dotted line

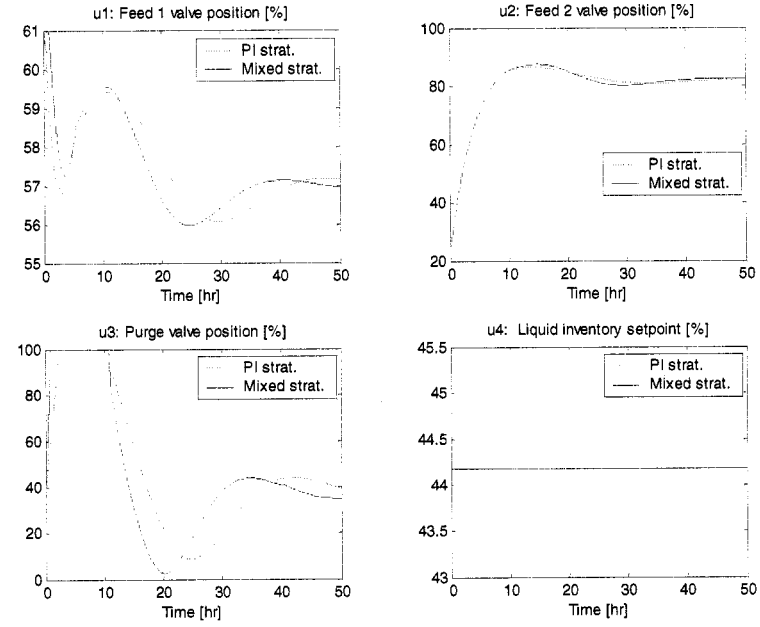

Figure 3.5: Scenario 1 – Manipulated variables – PI strategy (green) and mixed strategy (black)

Another example of this characteristic difference can be seen during scenario 2. An increase in production rate is demanded as quickly as possible, and in order to do so, pressure has to be increased from 2700 to 2850 kPa and y_{A3} has to increase from 47 to 63. In both strategies, setpoint changes are applied step-wise.

This is a relatively easy scenario but nevertheless, it is clear that PI performance is really poor (long settling time and large overshoots on P and y_{A3}). Step setpoint changes determine a quick increase in pressure; because of this, the override loop temporarily reduces production rate setpoint and then lets it rise smoothly.

Until about t=5 hr the two strategies follow the same pattern of response, but when pressure reaches its setpoint at 2850 kPa, the MPC loop quickly increases purge valve opening in order to mantain the desired value with a negligible overshoot. Once again, this is a consequence of the predictive nature of MPC.

Differently from scenario 1, where production and purge composition were not affected by the tighter pressure control, in this case some differences can be seen. A better tracking of pressure setpoint reduces the intervention by the override loop, and so a faster convergence to production setpoint is obtained. In fact, for the multiloop case the override structure has to intervene because pressure approaches dangerously to 2900 kPa; this determined a second decrease in production setpoint. Using MPC loop for pressure substantially reduces pressure overshoot, so production target can be reached more quickly.

A relevant improvement is also observable for purge composition: y_{A3} reaches its setpoint more quickly and with fewer oscillations. This too is a "side effect" of tighter pressure control.

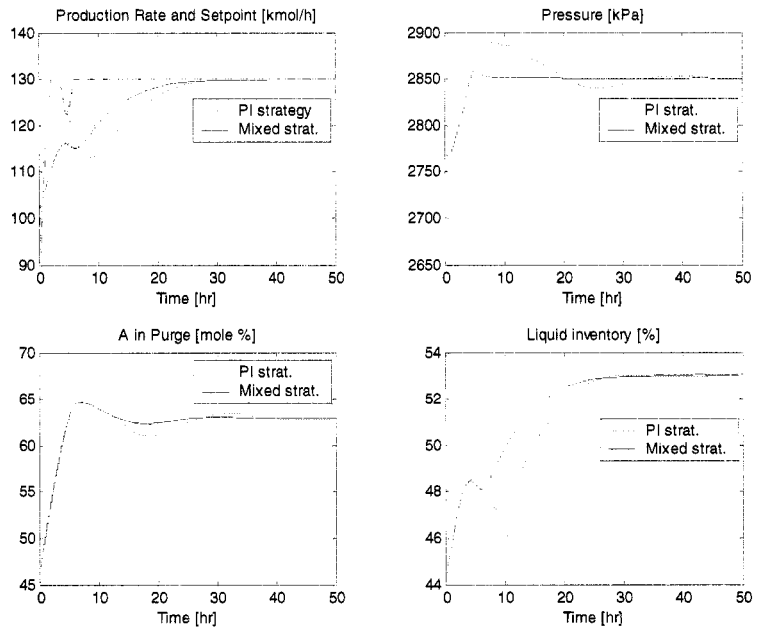

Figure 3.6: Scenario 2 – Controlled variables – PI strategy (green) and mixed strategy (black); production setpoint follows the same colours in a dotted line

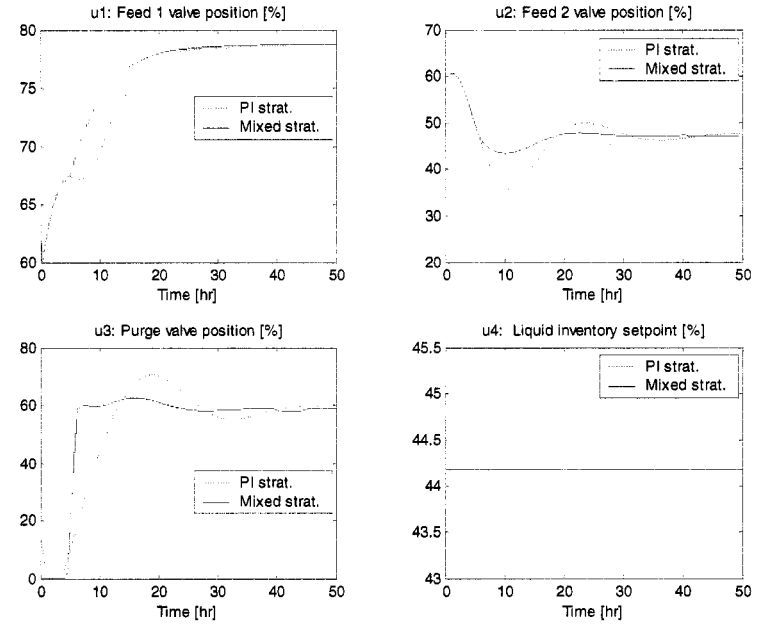

Figure 3.7: Scenario 2 – Manipulated variables – PI strategy (green) and mixed strategy (black)

In the following figures results from scenario 3 and 4 are presented together due to their similarities. Furthermore, both of them show how in some cases the nominal operating point is no longer possible.

For scenario 3, due to the sudden loss of Feed 2, not even purge composition setpoint is possible: in this case control on y_{A3} is completely lost. The latter phenomenon is a consequence of the SISO approach (if F_2 is not available, y_{A3} is uncontrollable) but also of the process structure (y_{A3} is minimally dependent on the other manipulated variables). This suggests that, regardless of the control strategy used, in scenario 3 purge composition is very difficult to control.

Furthermore, in both scenarios it is evident that the MPC loop gives almost no improvement. This is because the purge valve saturates very quickly and pressure control relies on pressure override. In these cases override structure is a key element and it determines most of the closed-loop dynamics (which is very similar for both strategies). However it must be recognized that MPC aggressiveness gives a minimal improvement, but it is just temporary.

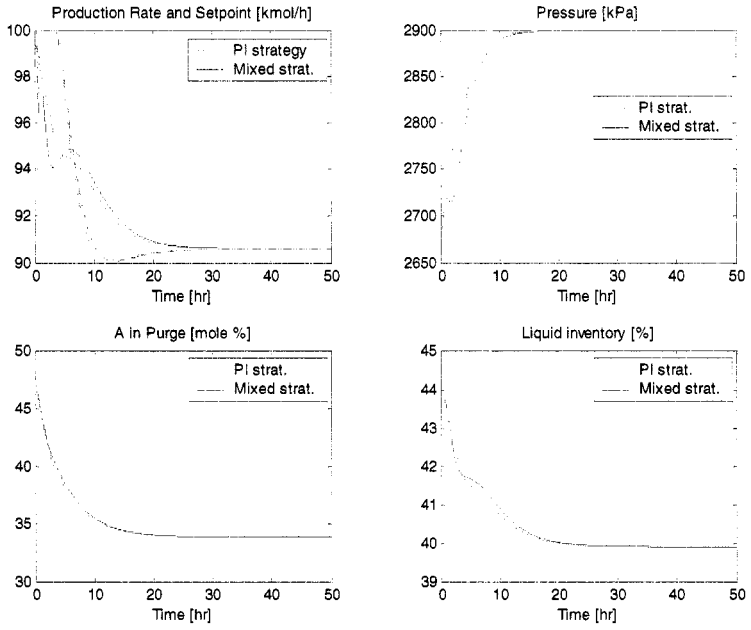

Figure 3.8: Scenario 3 – Controlled variables – PI strategy (green) and mixed strategy (black); production setpoint follows the same colours in a dotted line

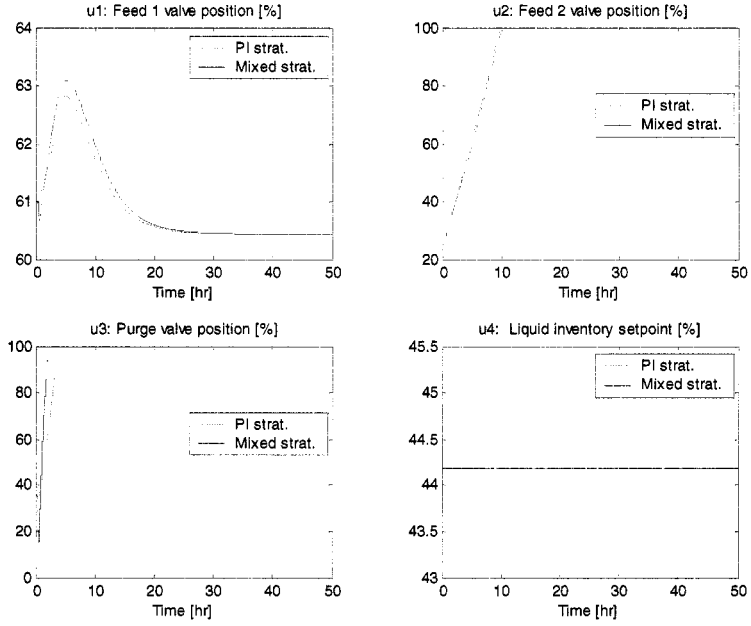

Figure 3.9: Scenario 3 – Manipulated variables – PI strategy (green) and mixed strategy (black)

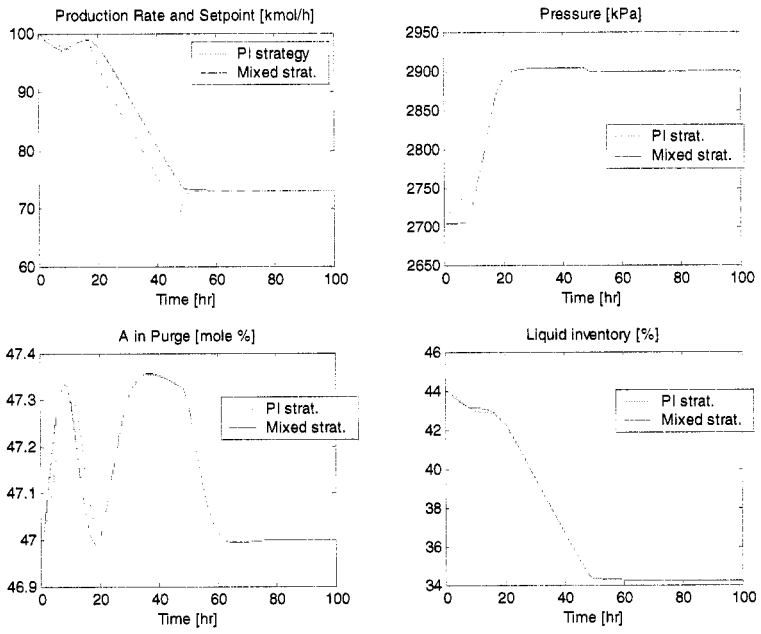

Figure 3.10: Scenario 4 – Controlled variables – PI strategy (green) and mixed strategy (black); production setpoint follows the same colours in a dotted line

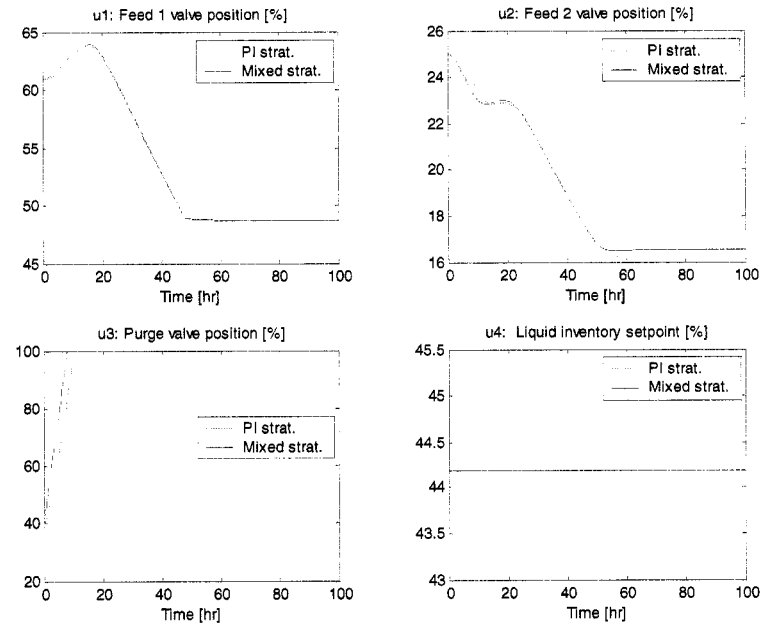

Figure 3.11: Scenario 4 – Manipulated variables – PI strategy (green) and mixed strategy (black)

In the case of a change on purge concentration setpoint (Scenario 5), y_{A3} has to increase from 47 to 63, while production and pressure must remain at their nominal value. This scenario presents behaviour similar to scenario 1, so it will not be discussed in detail.

Once again, pressure trajectory performance is limited by valve saturation, but as soon as pressure approaches 2700 kPa, the MPC quickly moves the purge valve in order to keep the controlled variable as close as possible to its setpoint.

Differently from scenario 1, in this case a tighter pressure control doesn't affect the trajectories for the other controlled variables. This is because the override structure doesn't give major corrections on production setpoint (only from t=0 to t=0.3 hours).

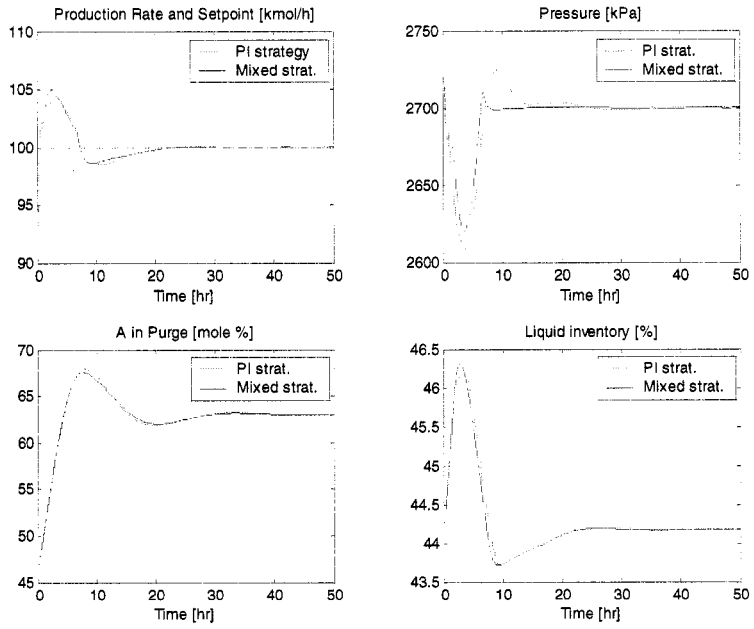

Figure 3.12: Scenario 5 – Controlled variables – PI strategy (green) and mixed strategy (black); production setpoint follows the same colours in a dotted line

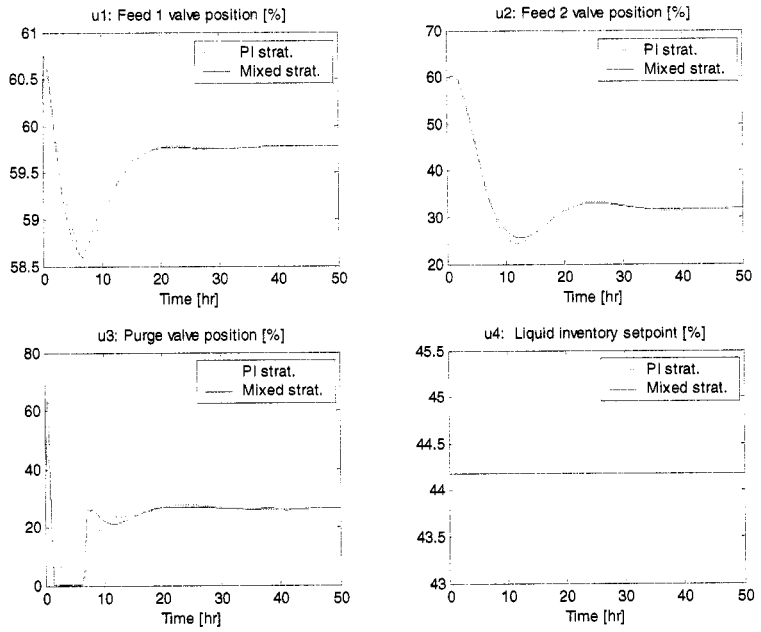

Figure 3.13: Scenario 5 – Manipulated variables – PI strategy (green) and mixed strategy (black)

Scenario 6 is an example of the possible improvement given by the MPC controller when no saturation problems arise.

An increase in inert content of Feed 1 is a minor disturbance and if uncontrolled it would result in a pressure increase (below shutdown limit) and minor variations on purge composition and product flow. The compensation of pressure rise is easily handled by opening purge valve without requiring the intervention of the override; chemical composition is easily adjusted by increasing Feed 2, and production rate is regulated by minor changes in Feed 1.

Although this is a relatively easy scenario, the MPC pressure loop gives much better performance than the PI loop used in Ricker (1993): a deviation from setpoint of only 5 kPa, rather than 25 kPa. This improvement is clearly obtained because of MPC's predictive behavior.

Again, production and y_{A3} responses do not show significant differences as a consequence of the introduction of the MPC controller.

In this case, since operating conditions are far from the constraints, it is reasonable to think that a well-tuned PID could give the same performance as the mixed strategy used.

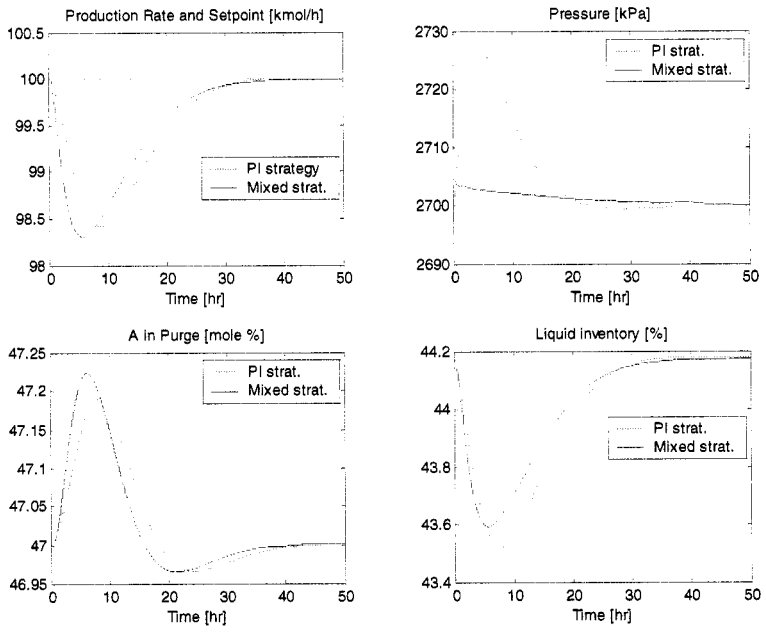

Figure 3.14: Scenario 6 – Controlled variables – PI strategy (green) and mixed strategy (black); production setpoint follows the same colours in a dotted line

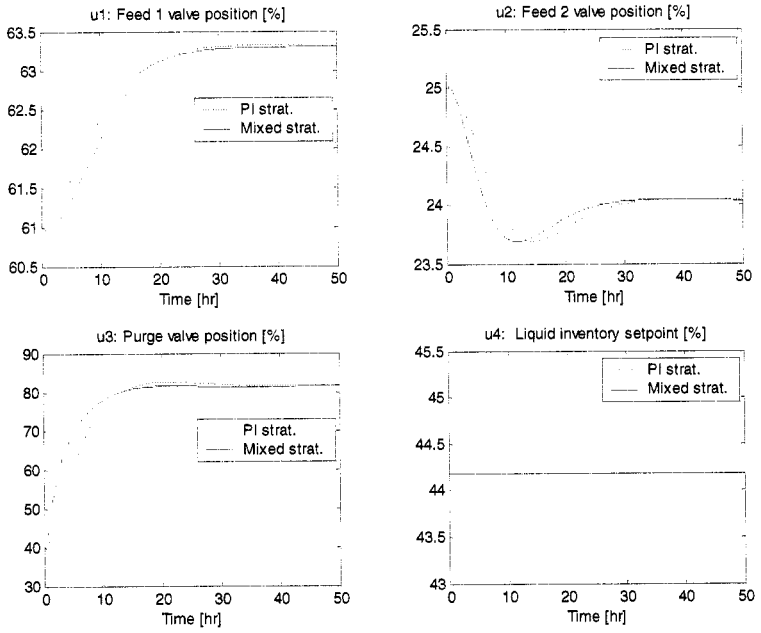

Figure 3.15: Scenario 6 – Manipulated variables – PI strategy (green) and mixed strategy (black)

3.2.7 Concluding remarks

Following the detailed analysis of the results obtained in the different scenarios, it can be stated that:

- MPC results in good improvement of pressure trajectory, but the improvement is limited by valve saturation
- As expected (according to system interactions), improvement on pressure loop generally doesn't affect production rate and purge composition trajectory
- Both multiloop strategies are very robust (no oscillation or stability problems), but performance suffers: even for easy scenarios (setpoint changes as in 2 and 5) settling times are long and overshoots are generally present

- More aggressive controller tuning could improve general performance, but most of the limitations are caused by the multiloop SISO approach.

Following these considerations, the next section will discuss attempts to overcome some of these limitations.

3.3 Multivariable Model Predictive Control

3.3.1 Motivation

In the last section a mixed multiloop strategy was shown and tested on the two-phase reactor under study and results were compared with the multiloop PI approach developed in Ricker (1993).

Even if the mixed strategy developed gave better results than multiloop PI strategy, in both cases performace was strongly limited by:

- valve saturation: constraints on the inputs are a key characteristic of this problem
- SISO approach: every controller operates indipendently and collaboration is not possible

This suggests that a multi-input multi-output (MIMO) strategy could overcome difficulties and, at least in theory, take advantage of the system interactions to have tighter control.

The selected approach is Model Predictive Control (MPC) due to its ability to handle constrained inputs and outputs.

3.3.2 The 4-by-4 system

The second attempt to improve the performance was to use a centralized MPC approach. This means that all the interactions of the considered system are taken into account and, at least theoretically, a centralized controller can take advantage of all interactions in order to maximize setpoint tracking. In particular, the MPC approach, because of its *optimality*, can lead to a minimization of output errors according to the priority given to each variable.

In this case, problems given by valve saturation would be decreased, because if one input is saturated, another one can be used to drive the most important output closer to its setpoint. Of course, this implies a larger error on one of the less important outputs.

This is theoretically very appealing, but it must also be considered that undermodelling errors, disturbances and shift in the operating conditions lead to error on trajectory predictions, thus limiting the actual performance of such a controller. MIMO MPC is also well known for robustness issues and for difficult tuning.

Prior to designing a MIMO MPC controller for the two-phase reactor considered, the portion of the system on which this approach is going to be implemented must be selected. The answer may seem obvious, but in reality it is not. In fact, a possible choice would be to use MIMO MPC on just one set of CVs and control others with another strategy. For example pressure (P) and product rate (F_4) could be handled in a centralized fashion using u_1 and u_3, while purge composition (y_{A3}) could be controlled by an independent controller manipulating u_2.

In order to leave full flexibility to the controller, a fully centralized strategy was chosen, meaning that the controller is allowed to handle the complete 4×4 system. As opposed to the mixed strategy shown before, the fourth manipulated variable (liquid inventory setpoint) is actually available for manipulation and liquid inventory is considered as an

output. This is explained by the following consideration: if liquid level in the reactor can be manipulated, temporary under- or over-production can be compensated.

For example, Figure 3.14, corresponding to scenario 6, shows that production rate decreases from 100 kmol/h to 98.5, or in scenario 1 (Figure 3.4) product flow floats between 93 and 103. In order to respond to these fluctuations, liquid inventory could be manipulated accordingly.

However, this modification has a major drawback: an excessive manipulation of liquid inventory can introduce oscillations in the system response and can even lead to instability problems. Oscillations result from the way liquid inventory is manipulated, that is through its setpoint (remember the presence of the P controller); this has a characteristic 'pulse' response on F_4 (as shown in Figure 3.16).
Stability problems may arise if liquid inventory approaches its constraints too closely. In this case, as discussed in Zafiriou (1991), hard constraints prevail on weighting factors.

3.3.3 Identification procedure

In order to implement centralized MIMO MPC a full model describing input-output relationships is needed. In the case considered of a four-by-four system, this leads to 16 SISO models.
As it is often the case for MIMO MPC a State-Space representation would be computationally more attractive. Nevertheless step response models were used following the procedure established with the mixed strategy, and also for the possibility of using the Matlab/Simulink MPC Toolbox.

Similarly to the SISO case, a step size and sign has to be chosen to test the plant. Once again, the trade-off is between capturing nonlinear dynamics and identifying the system around a given operating point. Since a step of -5% was chosen to obtain a step-reponse model for the SISO system, a consistent choice was made of ± 5% for all the manipulated variables. The response giving the higher gain was chosen for robustness reasons.

The following figure shows the results of all the ± 5% step tests. To create a better visual impact, the responses of all the interaction that were tested with a negative step are multiplied by -1.

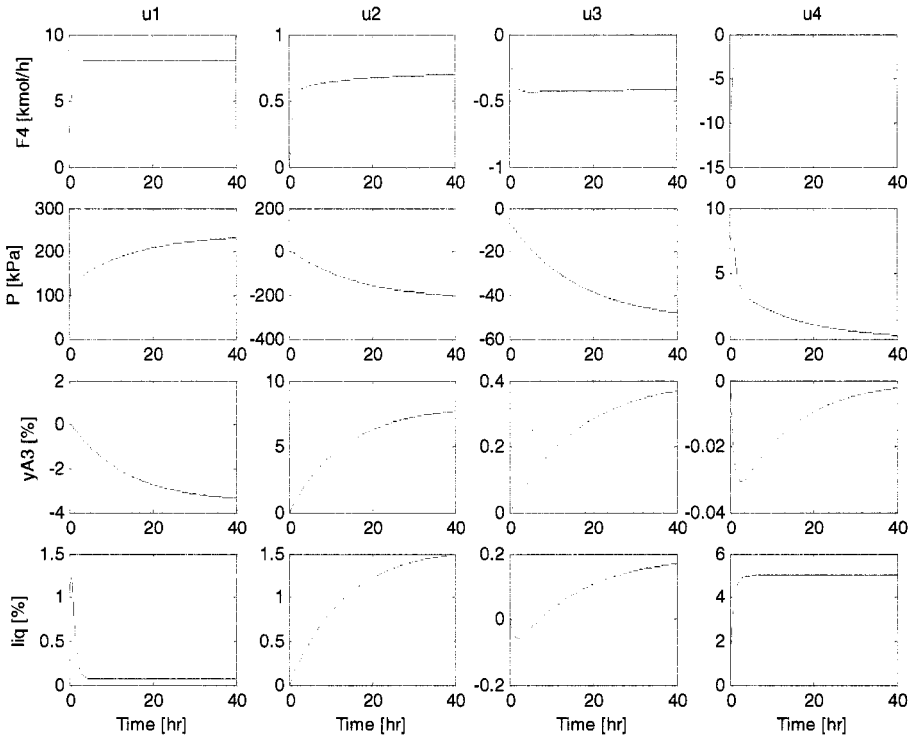

Figure 3.16: Step responses for the 4×4 system

It is clear that some interactions are much more important than others. For example it can be seen that:

- production rate (F_4 ; first row): effect by u_1 is one order of magnitude larger than u_2 or u_3; u_4 has a temporary but significant influence
- pressure (P; second row): u_1 and u_2 have larger influence than u_3, as expected; contribution by u_4 is temporary and minimally important
- purge composition (y_{A3}, third row): u_2 has the most important effect; u_3 and u_4 are negligible
- liquid inventory (*liq*; fourth row): for obvious reasons u_4 is the most influential input with a gain equal to 1

It is important to point out the characteristic behavior of the first three elements of the fourth column. These correspond respectively to the product flow (F_4), pressure (P) and purge composition (y_{A3}) responses following a step change of +5% on the liquid inventory setpoint. It is easy to understand that liquid inventory doesn't affect the final steady state for these outputs, but there is still a transient time over which a deviation from the nominal value is present.

The importance of this behavior is totally negligible for purge composition because the new inventory setpoint is reached very quickly while composition dynamics are very slow. The effect on pressure is not as small as for purge composition, but compared to the gains given by u_1, u_2 and u_3, it can be easily neglected.

The case of production rate (F_4) is different: this is because product flow is the manipulated variable for the built-in P controller on liquid inventory. A setpoint change on liquid inventory implies a temporary change in F_4 in order to reach the desired value of liquid inventory. In this case the deviation from nominal values is quite important and occurs quickly; this 'pulse like' response has important consequences on the global system, notably it can cause some high-frequency low-amplitude oscillations on the product flow.

The last response is not surprising at all since liquid inventory is an integrating process regulated by a proportional controller; this gives approximately a first order dynamics with zero offset.

Since step response was also used for the MIMO MPC approach, model coefficients $[s_1, s_2, ...s_N]$ could be obtained sampling actual plant output. Nevertheless 16 transfer functions fitting each one of the above presented responses were found. The goal of this procedure was to have a simplified, linear model for the plant at the nominal operating point. This reduced model was also used for preliminary test of each control strategy. Another advantage of having such a model is that in the simulations model length can be changed very easily.
This procedure could be performed quite easily and with a very good quality. In the Appendix a table with the identified 16 identified transfer functions can be found.

3.3.4 Tuning parameters

As already mentioned, one of the major difficulties of MIMO MPC is its tuning; as it was the case for the SISO approach, tuning of MPC is the choice of the parameters of the open-loop optimization. The only difference is that for the multi variable case, the number of parameters increases largely.

For the fully centralized approach (4×4 system) the parameters to be tuned are:

- T, sampling time for MPC
- n, model length
- P, prediction horizon
- M, control horizon
- Λ_y, output weighting (4 values)
- Λ_u, control action weighting (4 values)

This gives a total of at least 12 values. Moreover, some generalization could be introduced: different Ms and Ps for each variable, variable weighting factors, blocking factors and constraint softening are just some examples. This gives an idea of the huge number of possible choices. See Maciejowski (2002) for details in this sense.

In order to reduce the complexity of the problem the following decisions were made:

- fixed, constant prediction horizon for all outputs
- fixed, constant control horizon for all inputs
- constant output and input weights
- no blocking factors

Sampling time was fixed to 0.1 hr for consistency with the composition measurement period (6 minutes). A model length of 400 (corresponding to 40 hrs) was chosen in order to have most of the step response models representing at least 90% of the gains. Errors on the last step response coefficients for the 16 SISO models are shown in the following table:

Table 3.3 : Error on final gain

	u_1	u_2	u_3	u_4
F_4	1.2e-013%	1.2%	-0.28%	1.53e-12 *
P	3.4%	8.8%	8%	5.83e-2 *
y_{A3}	5.2%	5.2%	8.8%	-4.64e-4 *
liq	1.7e-012%	5.2%	13%	1e-013%

* absolute errors

It can be observed that almost all the approximations are good: the only one with a gain error greater than 10% is liq/u_3, but this transfer function has minor importance in the system.
Note that in Table 3.3 some values of the fourth column are absolute errors. For these cases relative errors are not very meaningful since these responses have gains equal to zero.

For prediction and control horizon the same considerations made for the SISO case are still true. The only difference is that for the MIMO approach computational effort can quickly become an issue if parameters are not chosen properly.
A final choice of M=10 and P=60 was judged a good trade-off between performance and computational effort.

All the parameters discussed up to this point are not especially critical for closed-loop stability and performance. On the contrary, input and output weights proved to be crucial for the overall behaviour of the controlled system. All this suggests that particular care should be exercised for this choice.

A possible approach to select weights could be according to the priority assigned to each variable as a consequence of its importance for the treated system. Weighting factors are assigned to controlled variables according to process and economic considerations while manipulated variables are penalized according to the smoothness desired and possibly their costs.
In the application under study this leads to the selection of 8 parameters; which makes the tuning quite complex.

In order to simplify the tuning procedure, a systematic procedure to select MV weights was used.

Inputs

In order to simplify the tuning process, the following systematic procedure was used to select MV weighting factors. Given a choice of output weights, an indication of the penalties to be assigned to the inputs is given by the the analysis of the following matrix:

$$\Omega = \underline{\underline{\beta}}^T \underline{\underline{\Delta}}_y \underline{\underline{\beta}} \tag{3.8}$$

where $\underline{\underline{\beta}}$ is the "dynamic matrix" for the MIMO system (see section 3.1.2) and matrix Ω is part of the solution of the uncostrained optimization problem given in Ogunnaike (1994):

$$\Delta u_{OPT} = \underline{\underline{\beta}}^T \underline{\underline{\Lambda}}_y \underline{\underline{\beta}}(1 + W\underline{e}) \tag{3.9}$$

The importance of matrix Ω comes from the fact that the main diagonal of Ω gives an indication of the *global* influence of each manipulated variable on the weighted outputs. Weights for controlled variables were assigned according to the average of the elements on the main diagonal. Extra penalty could also be added or removed by manually adjustung some of the results obtained by this procedure. Moreover, a scaling factor λ_u can be added for robustness reasons (i.e. to increase smoothness of input manipulation):

$$\Lambda_u = \lambda_u \frac{1}{M}\left[\sum_{i=1}^{M}\Omega_{i,i} \quad \sum_{i=M+1}^{2M}\Omega_{i,i} \quad \sum_{i=2M+1}^{3M}\Omega_{i,i} \quad \sum_{i=3M+1}^{4M}\Omega_{i,i}\right] \tag{3.10}$$

By this procedure, given a set of weights for CVs, values for MVs can be automatically calculated. For the application under study this implies the selection of only 4 parameters.

Outputs

Process and economic consideration for the two-phase reactor under study would lead to an increase of the weighting for the production rate and purge composition, and relaxation the ones for pressure and liquid inventory. This logic works very well in theory but conceals some problems.

Some simulations were run trying to maximise production and possibly purge composition, while a certain freedom was left for pressure and liquid inventory (input weights were calculated according the above procedure). This leads to the same problems described in Ricker (1993): unacceptable performance (oscillations) or even unstable behaviour.

The reason for such behaviour was identified in the excessive importance given to certain variables and consequently the excessive freedom for pressure and liquid inventory. In most cases these were likely to get too close to the constraints assigned. This fact introduces large oscillations since hard constraints prevail on weighting factors (as explained in Zafiriou, 1991).

Another important factor determining unstable behavior is found in the gain sign inversion presented by P/u_2. In fact in some cases y_{A3} is *sacrificed* in order to keep pressure below its constraint by means of u_2. This decision is consistent with the gain identified around nominal operating point for this interaction (high and negative), but in different conditions it has an effect opposite to the expected one. In such circumstamces pressure diverges.

These observations lead to the conclusion that weights of variables with active contraints should be increased to avoid excessive fluctuations and to enforce constraint satisfaction. This is particularly valid for liquid inventory because of the dramatic consequences of its oscillations. Furthermore a relatively high priority must be given to purge composition in order to prevent pressure control by means of u_2.

The following table summarises the values for the parameters discussed:

Table 3.4 : Tuning parameters for the proposed multivariable MPC strategy

Parameter	Significance	Value
T	Sampling time	0.1 hr
P	prediction horizon	60
M	Control horizon	10
Λ_y	Output weighting factor	[1; 0.09; 2; 2.1]
Λ_u	Input weighting factor	[3.9; 0.19; 0.036; 0.065]
λ_u	Robustness scaling factor	2

It is necessry to mention a few considerations on the resulting choice of input weights. It is important to note the fact that the weights obtained throught the systematic procedure described above are consistent with the effect of each manipulated variable and the weights assigned to the controlled variables. For example u_1 has a high penalty because of its strong influence on the system (especially production rate and pressure); or also, u_3 has the lowest penalty since it affects only pressure (low priority) and with a relatively low gain. Thus it can be conluded that the systematic procedure for choosing input weights gives reasonable results.

3.3.5 Results for MIMO MPC

The MIMO approach described was tested on Matlab/Simulink simulations. Here the results found are shown and discussed briefly. Control preformance of MIMO MPC control structure is compared with multiloop PI approach and mixed strategy. For these,

production rate setpoint (adjusted by pressure override) is not shown here for clarity reasons. Further details on this aspect can be found in previous sections.

It would be also interesting to compare the performance given by the MIMO MPC strategy proposed here with the performance obtained through the centralized and decentralized strategies of Ricker (1993). This comparison was not performed since reproducing the results of Ricker (1993) was not the main focus of this work.

In Figure 3.17 and Figure 3.18 results for Scenario 1 are presented. It is evident how the MIMO structure greatly improves control performance for all the controlled variables. Production rate and pressure are the most affected, since a very small deviation from setpoint is obtained.

This result is obtained through a synergy of the control moves. As the perturbation enters the system, y_{A3} and the production rate tend to drop while pressure tends to increase greatly. A drop in y_{A3} is contrasted through a quick increase in Feed 2 valve opening (u_2), while pressure is handled by a combined increase in u_3 and decrease in u_1; as soon as pressure stops its rise, u_3 is desaturated and the system is slowly but efficiently settled to its nominal output values.

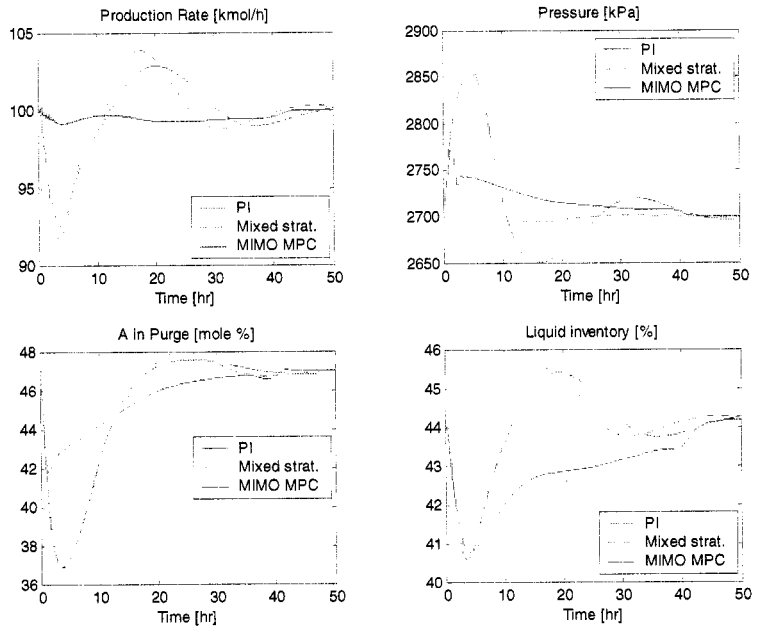

Figure 3.17: Scenario 1 – Controlled Variables – PI strategy (blue dashed), mixed strategy (red dotted) and MIMO MPC (black solid)

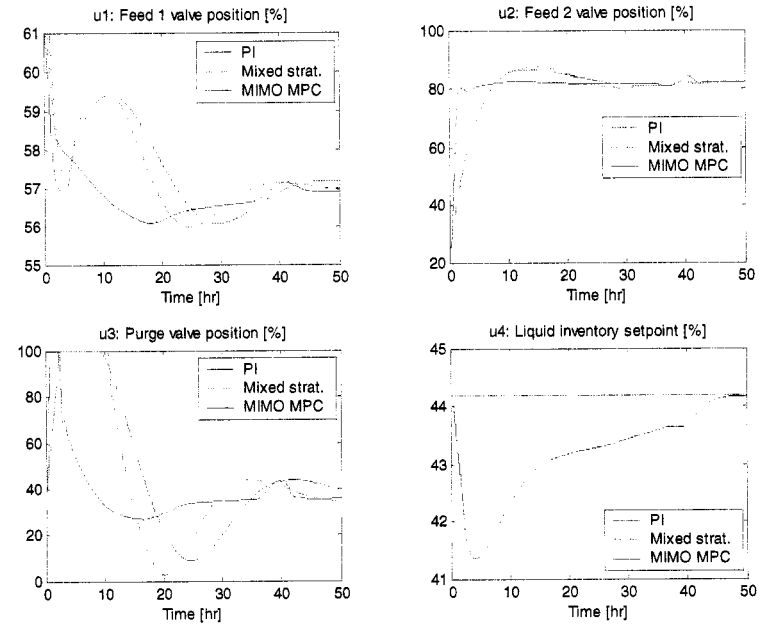

Figure 3.18: Scenario 1 – Manipulated Variables – PI strategy (blue dashed), mixed strategy (red dotted) and MIMO MPC (black solid)

Figure 3.19 and Figure 3.20show results found for Scenario 2 (increase in production setpoint and consequently also in pressure and y_{A3} setpoints).

In this case MIMO MPC shows a great ability to track setpoint changes using its predictive nature. The desired reference trajectory is a first order with time constant of 2.4 hours for all the outputs.

Analyzing control actions, it can be observed that u_2 presents a large 'overshoot' and then it settles to its steady-state value; this occurs since purge composition dynamics are very slow compared to the demanded closed-loop dyanmics and so an aggressive control action is required. Feed 1 valve position presents a pattern similar to the mixed strategy, but here u_1 is moved more aggresively resulting in a faster convergence. Also remember that for mixed strategy, pressure override greatly affected production setpoint.

Purge valve (u_3) is completely opened to limit the predicted pressure increase given by the fast opening of u_1, and then it is used to track pressure setpoint.

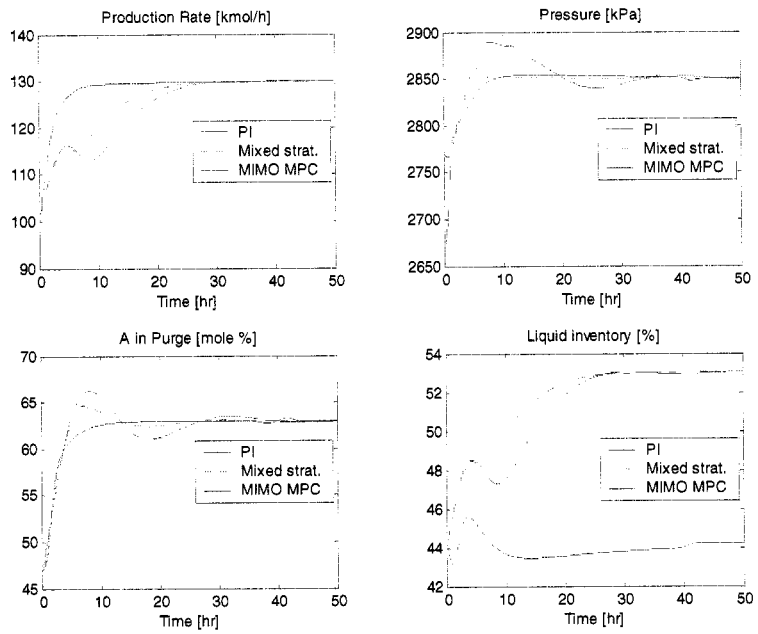

Figure 3.19: Scenario 2 – Controlled Variables – PI strategy (blue dashed), mixed strategy (red dotted) and MIMO MPC (black solid)

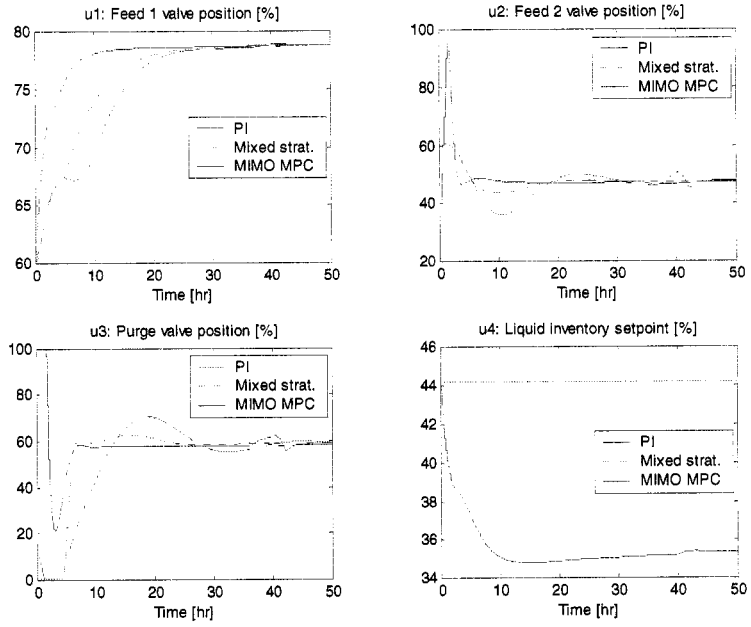

Figure 3.20: Scenario 2 – Manipulated Variables – PI strategy (blue dashed), mixed strategy (red dotted) and MIMO MPC (black solid)

In the following figures results from scenario 3 and 4 are presented; these results are discussed together since they present similar characteristics. In both of these scenarios the starting operating point is no longer feasible, so some freedom is left to MIMO MPC in determining which operating point is the best. This is done according to the weights assigned to each variable.

In these scenarios it is clear how the choice of weighting factors influences the closed-loop behavior. In fact, in this case product flow could be kept much closer to 100 kmol/h using liquid holdup in the reactor but the weights chosen make this impossible since liquid inventory has a higher priority than production rate.

In section 2.2.2 it was said that scenario 3 and 4 must be considered as highly demanding. This is not due to the speed with which the disturbance affects the system, but rather by the large deviation from the original operating point necessary. This aspect is not relevant for a decentralized approach, but it has important consequences on the MIMO MPC strategy. In these scenarios it was observed that a low penalty for liquid inventory results in a constraint violation that causes important oscillations.

For obvious reasons, in the case of sudden loss of F_2 (scenario 3) purge composition control is lost. But it is important to note that this disturbance is easily detectable, since the measurement of Flow 2 is available.

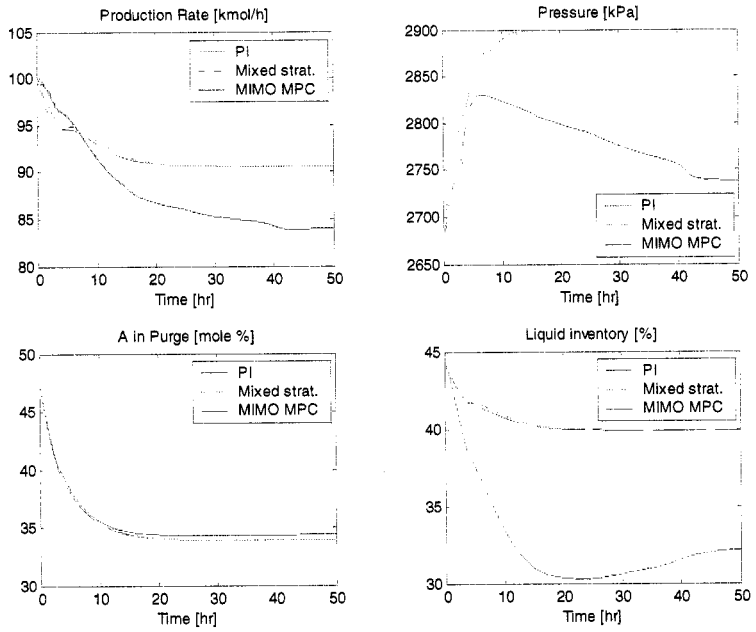

Figure 3.21: Scenario 3 – Controlled Variables – PI strategy (blue dashed), mixed strategy (red dotted) and MIMO MPC (black solid)

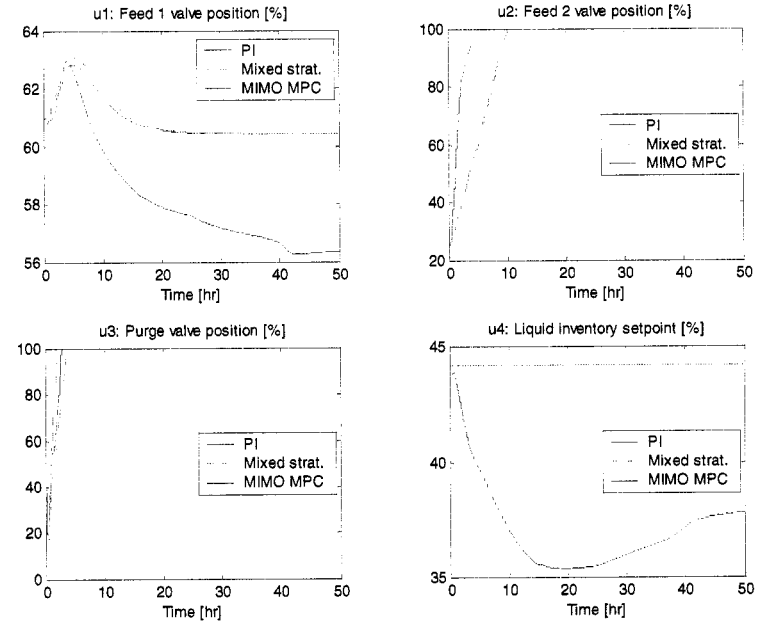

Figure 3.22: Scenario 3 – Manipulated Variables – PI strategy (blue dashed), mixed strategy (red dotted) and MIMO MPC (black solid)

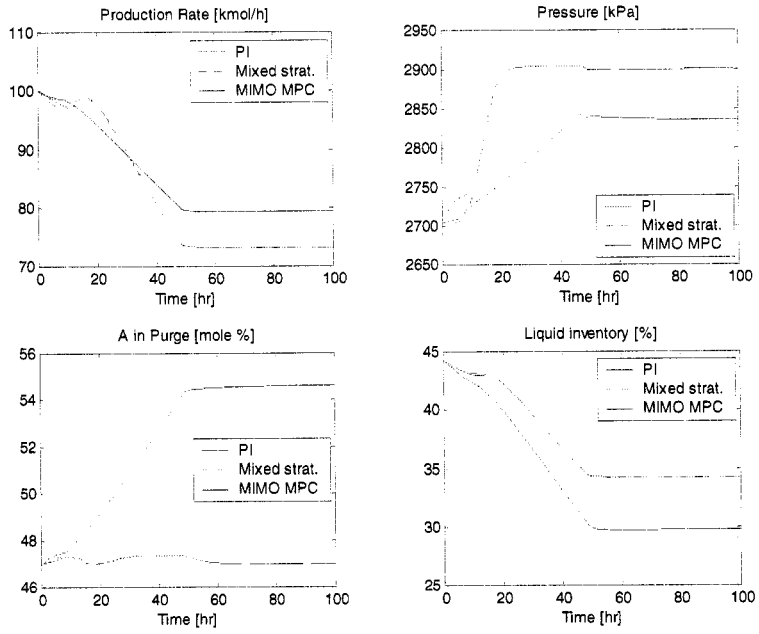

Figure 3.23: Scenario 4 – Controlled Variables – PI strategy (blue dashed), mixed strategy (red dotted) and MIMO MPC (black solid)

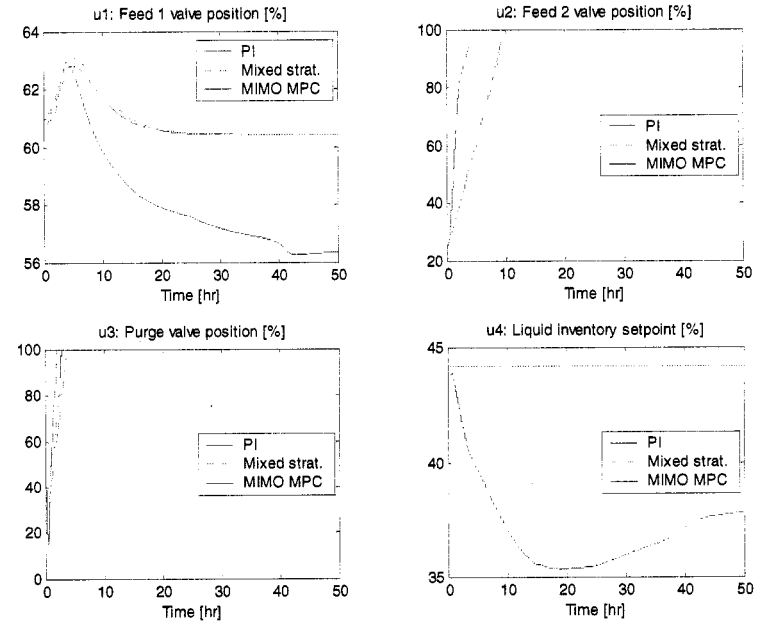

Figure 3.24: Scenario 4 – Manipulated Variables – PI strategy (blue dashed), mixed strategy (red dotted) and MIMO MPC (black solid)

In Figure 3.25 and Figure 3.26 results from scenario 5 are shown. In this case a setpoint change in purge composition is required, while other setpoints remain at their nominal value. The reference trajectory is first order with time constant of 2.4 hrs.

Pure A feed (u_2) is moved much more aggressively than with previous control structures in order to track composition setpoint. Once again, this behavior is a consequence of the predictive nature of MPC. Because of the output weights chosen, a deviation from production rate of 100 kmol/h is tolerated in order to have a better tracking of purge composition. Purge valve is suddenly closed to respond to the expected drop in pressure given by the movement of Pure A feed valve, while Feed 1 control actions are more difficult to understand.

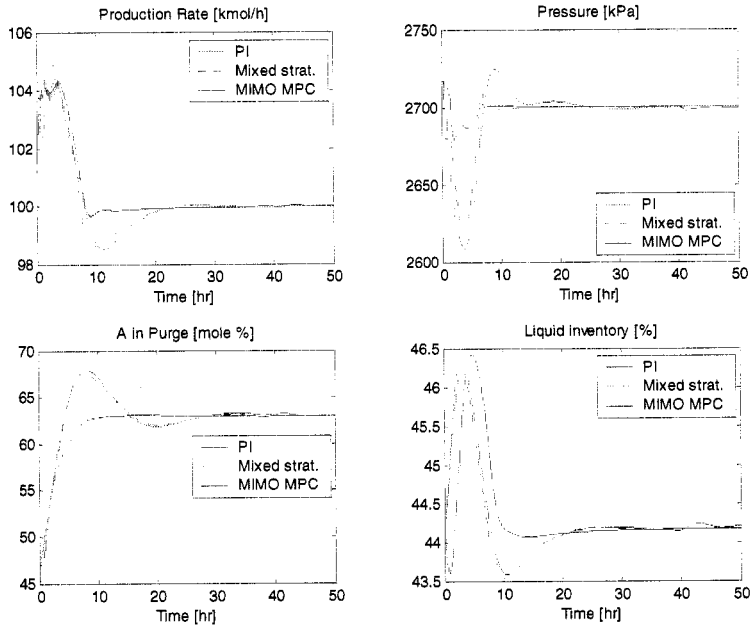

Figure 3.25: Scenario 5 – Controlled Variables – PI strategy (blue dashed), mixed strategy (red dotted) and MIMO MPC (black solid)

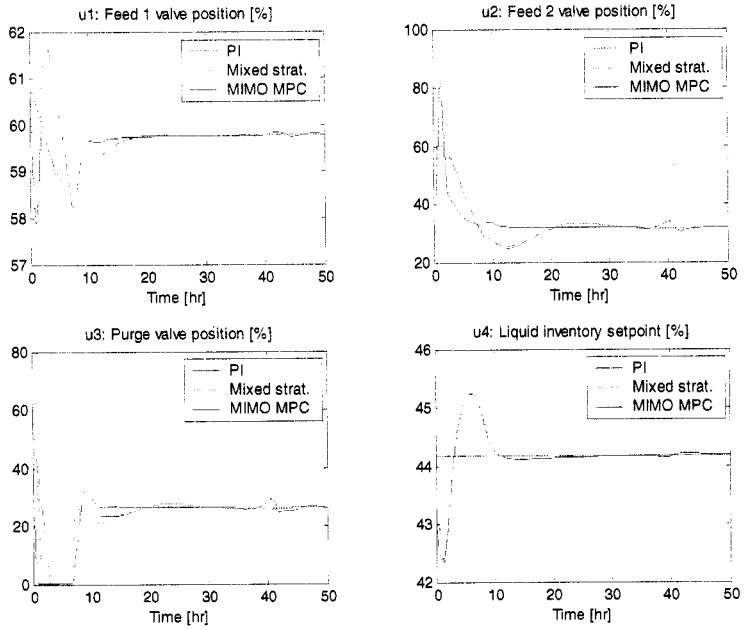

Figure 3.26: Scenario 5 – Manipulated Variables – PI strategy (blue dashed), mixed strategy (red dotted) and MIMO MPC (black solid)

Results from scenario 6 are shown in Figure 3.27 and Figure 3.28. In this case MIMO MPC gives a substantial improvement in performance without particular differences in the patterns followed by the manipulated variables. The improvement is mainly given by more direct and incisive control actions, consequence of the predictive nature of MPC.

In this case it is important to note how liquid inventory setpoint (u_4) is used to help u_1 in responding to a drop in product flow. This feature could be used more aggresively by assigning a lower weight to liquid inventory but, as said before, this causes instability problems in other circumstances.

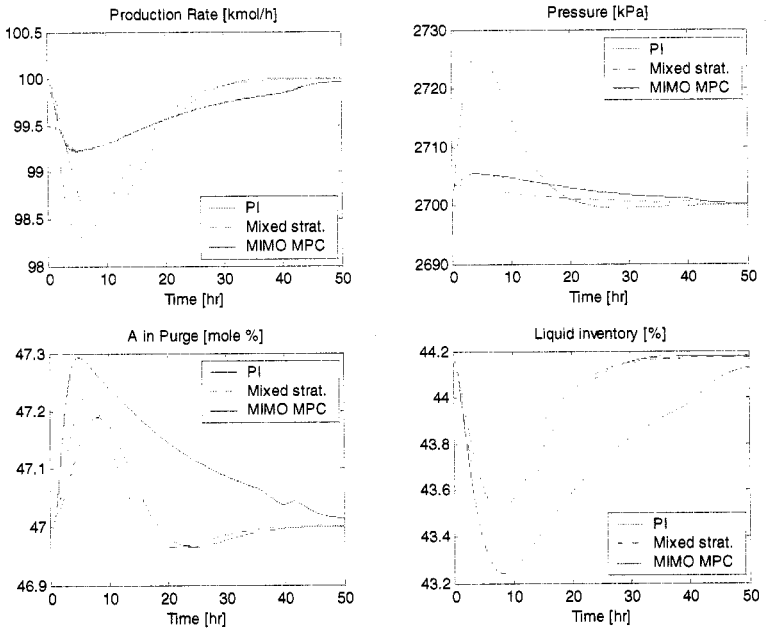

Figure 3.27: Scenario 6 – Controlled Variables – PI strategy (blue dashed), mixed strategy (red dotted) and MIMO MPC (black solid)

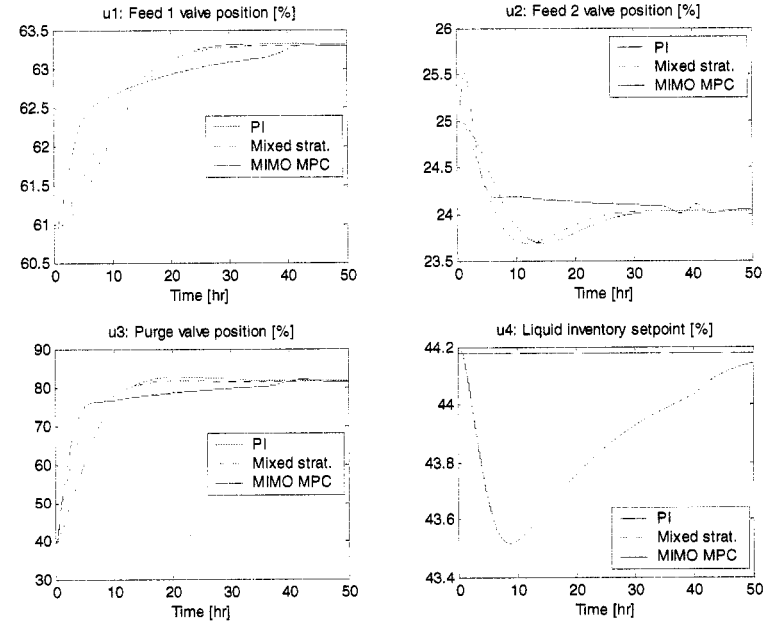

Figure 3.28: Scenario 6 – Manipulated Variables – PI strategy (blue dashed), mixed strategy (red dotted) and MIMO MPC (black solid)

3.3.6 Differences between the proposed multivariable MPC and Ricker (1993)

At this point, it is important to point out what the main differences are between the centralized strategy of Ricker (1993) and the centralized strategy proposed in the last few sections.

First of all, the model incorporated in the MPC controller is different because in Ricker (1993), a continuous-time, linear, state-space model is used; this is obtained through a linearization of the nominal model of ordinary differential equation. On the other hand, in the work of this thesis step response models of the 16 transfer functions were obtained through a more empirical methodology, i.e. step tests on the manipulated variables.
The choice of Ricker (1993) is consistent with the use of an MPC structure based on a state-space representation, but it assumes perfect knowledge of the system, which is not generally the case in a real setting.

The second major difference is given by the different tuning of the MPC controller. In Ricker (1993) weight of input and output variables (CVs and MVs) are chosen only according to process and economic considerations. This leads to high weight values for production rate (F_4) and purge composition (y_{A3}), while pressure (P) and liquid inventory are assigned low weights. This works very well in theory, but it leads to instability because of the high model mismatch. As pointed out in Ricker (1993) stability problems arise in particular when the constrained variables approach their constraints.
On the other hand, in the work of this thesis other considerations were taken into account. First of all, higher weights were chosen for the constrained variables (P and *liq*) in order to avoid an excessively loose control and the consequent stability issues. Furthermore, as explained in section 3.3.4, purge composition priority was increased in order to highly penalize the use of the troublesome transfer function P/u_2. Also,

weights for the MVs were chosen according to a systematic procedure (see section 3.3.4), in order to decrease the complexity of the tuning.
Some other differences in the tuning parameters were also observed (sampling time, prediction and control horizons, blocking factors, etc.) but it is believed that these do not concur significantly to the different closed-loop performances obtained.

3.3.7 Concluding remarks

A MIMO MPC strategy greatly improved the overall performance of the reactor during the six scenarios tested. The reasons for such improvement can be identified in:

- MIMO approach: manipulated variables are used synergically, and system interactions are exploited; also, the manipulation of liquid inventory allows faster compensation of temporary production fluctuations
- MPC optimality and predictive nature: the system model is used to predict the best input trajectory; control actions are 'aggressive' and rapid; this aspect greatly improved performance for setpoint changes

Nevertheless some difficulties have been encountered:

- Tuning poses some problems due to the large number of parameters to be selected; a systematic procedure was developed for input penalty; the choice of output weights was determined more by stability considerations than by variable priority.
- Some stability issues arose; this is especially related to constraint violation and by system nonlinearities; however proper tuning could solve these problems.

Some of the problems are caused by the fact that the process is strongly nonlinear and the model used by MPC is fixed and assumed linear. Illustrative in this direction is the

example of the gain sign inversion for P/u_2 transfer function: process gain inversion in sign determines an unstable closed-loop system.

This naturally suggests the need for using adaptive techniques to improve control performance.

CHAPTER 4 Adaptation

In the last chapter it was shown that performance of the MIMO MPC strategy was limited, among the other factors, by large plant-model mismatch resulting from the strong nonlinearities of the system. In particular, the gain sign inversion presented by P/u_2 transfer function proved to be critical.

One of the possible solutions to these problems is represented by model adaptation techniques. In fact, since MPC is a model based approach, an improvement of the the model known by the controller, would give an output prediction closer to reality and consequently 'better' control actions could be taken. The basic concept of this approach is shown in Figure 4.1.

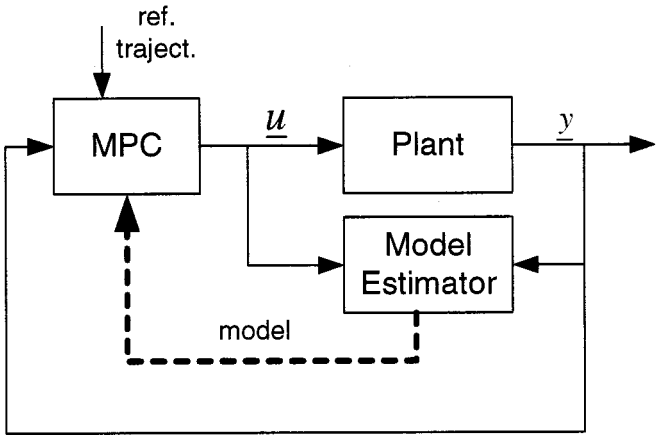

Figure 4.1: Indirect adaptive scheme for Model Predictive Control

All 16 transfer functions of the system present large gain variations over the different operating conditions. Nevertheless P/u_2 presents the most critical change: a gain sign inversion; this greatly limited performance obtainable by MPC and forced the selection of weighting factor on purge composition.

Following these considerations, an attempt to adapt pressure dynamic model will be shown. The first approach concerns P/u_2 only, following which a multivariable adaptation strategy will be presented. The controller used is the multivariable Model Predictive Control developed in the previous chapter. Two different techniques were tested: Model Weighting Adaptation (MWA) and Recursive Least Square Adaptation (RLSA).

4.1 Overview on Model Weighting Adaptation

Model Weighting Adaptation is an adaptation algorithm where the process model is computed as a linear combination of a set of possible plant models. These are simple First Order plus Dead Time (FOPDT) with gain and delays belonging to predetermined ranges. This implies that, differently from other adaptation algorithms, some *a priori* knowledge is necessary.

Model Weighting Adaptation is used in the industry for its very simple and yet powerful approach. The main advantage of this algorithm from an industrial point of view is its simplicity: no special computations are needed and it can be easily implemented in most DCS systems. Furthermore the boundedness of gains and delays results in a reasonable identified model (i.e. no unstable models or unrealistic gains are identified).

The main drawback is that undermodelling errors, high noise-to-signal ratio or disturbances badly affect model identification. Furthermore under certain circumstances proper model identification is not possible.

4.1.1 Prior knowledge

In order to build the model family model necessary to implementing MWA, some prior knowledge of the process has to be obtained. In particular gain and delays ranges have to be determined.

As previously mentioned, a model family is composed of a set of FOPDT transfer functions. Since MWA is a discrete-time algorithm, family members have to be expressed as:

$$P_{i,j}(z^{-1}) = g_i \frac{1-\alpha}{1-\alpha z^{-1}} z^{-d_i-1} \tag{4.1}$$

with: $g_i \in G = [g_1, g_2, \ldots g_{L_g}]$ where G is a partition of the gain range

$d_i \in D$ where D is the interval of possible delays expressed as multiples of the sampling time

Finally the family F of possible models can be expressed as:

$$F = \left\{ g \frac{1-\alpha}{1-\alpha z^{-1}} z^{-d-1} \middle| g \in G \times d \in D \right\} \tag{4.2}$$

4.1.2 Weight computation

The weight for each member of the family model is computed according to the error on the plant output given by that particular model. If the familiar truncated 2-norm is used, error for model P_{ij} it is obtained by:

$$\left\| e_{ij}(t) \right\|_{2,\lambda}^2 = \sum_{k=0}^{t} \lambda^{t-k} e_{ij}^2(k) \tag{4.3}$$

Note that a forgetting factor is added in order to give more importance to new measurements.

Weights are calculated as the normalization of the inverse of the errors, that is

$$w_{ij}(t) = \frac{\left(\mu + \left\| e_{ij}(t) \right\|_{2,\lambda}^2 \right)^{-1}}{\sum_{l,m} \left(\mu + \left\| e_{ij}(t) \right\|_{2,\lambda}^2 \right)^{-1}} \tag{4.4}$$

It is important to point out that a very small positive constant μ is added in order to prevent any possible division by zero. Other more refined techniques are possible to avoid this problem, such as introducing an error threshold, but they were not considered in this work.

4.1.3 The resulting Model

Once weights are calculated, the resulting total model can be computed as the linear compositon of the N models member of the model family:

$$P_m(z^{-1}) = \sum_{i=1}^{L_g}\sum_{j=1}^{L_d} w_{ij}P_{ij} = \sum_{i=1}^{L_g}\sum_{j=1}^{L_d} w_{ij}g_i \frac{1-\alpha}{1-\alpha z^{-1}} z^{-d_j-1} P_{ij} = \frac{1-\alpha}{1-\alpha z^{-1}} \sum_{j=1}^{L_d} \gamma_j z^{-d_j-1} \quad (4.5)$$

$$\gamma_j = \sum_{i=1}^{L_g} w_{ij} g_i \quad (4.6)$$

An important factor is represented by the weight map sharpness. This indicates how close the identified model is to the actual plant. This parameter is easily computed online by the following equation:

$$W(t) = \sum_{ij} \sqrt{w_{ij}(t)} \quad (4.7)$$

The remarkable property of this measure is that it is bounded between 1 (perfect fit) and $\sqrt{N}$, where N is the number of models belonging to the family. A value of $W(t)$ close to its upper bound means that the algorithm is not able to discriminate between the family members.

Furthermore, in order to reduce the effect of steady-state offset and disturbances, it is desirable to filter input/output data. Obviously the type of filter used plays an important role in the identification obtained; for the work of this thesis the first difference filter $(1-q^{-1})$ was used.

4.1.4 Additional features of the algorithm

What has been presented up to this point represents the base MWA algorithm. In order to improve performance, some additional features are possible, particularly in order to treat undermodelling errors. These are biefly mentioned here since they were not used in the work of this thesis. Further details can be found in Gendron (1998).

The first possible attempt to increase performance is to lock good model estimates. In fact, as perturbations enter the system, or signal-to-noise ratio decreases, the map weights tends to uniformity. One of the possible approaches to avoid this is to update the model estimate only when this is characterized by lower weight map flatness (W).

Furthermore, bad identification of the plant may occur because of undermodelling errors. As it shown in Gendron (1998), systems with very similar step responses can give quite different results with the MWA algorithm. In particular, unmodelled dynamics can largely reduce weight map sharpness. The easiest way to correct this problem is to apply a proper filter to the input/output data.

4.2 Recursive Least Square Adaptation

In the following sections an indirect adaptive algorithm will be presented. The approach used is the well known Recursive Least Squares (RLS) algorithm, which is based on the scheme shown in Figure 4.2. Details can be found in Landau *et al.* (1998).

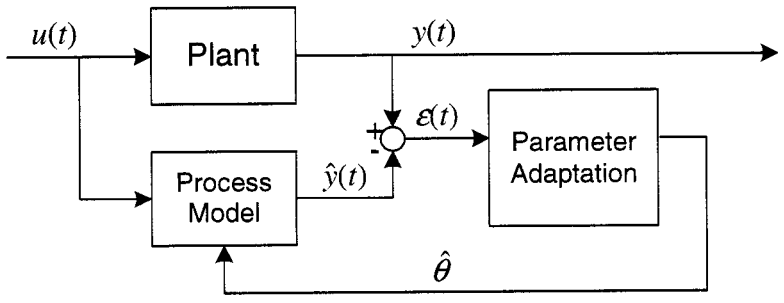

Figure 4.2: Parameter adaptation scheme

4.2.1 The Regression Model

The discrete-time model for the process can be expressed by:

$$y(t) = -\sum_{i=1}^{n_A} a_i y(t-i) + \sum_{i=1}^{n_B} b_i u(t-d-i) \tag{4.8}$$

where t represents the sampled time, $y(t)$ is the output, $u(t)$ is the input, d is the system delay expressed in sampling times, and a_i and b_i are the parameters of the model.

Using the backward shift operator $q^{-1}y(t) = y(t-1)$, the following relationships hold:

$$1 + \sum_{i=1}^{n_A} a_i q^{-i} = A(q^{-1}) = 1 + q^{-1}A^*(q^{-1}) \tag{4.9}$$

where: $A(q^{-1}) = 1 + a_1 q^{-1} + \ldots + a_{n_A} q^{-n_A}$ (4.10)

$$A^*(q^{-1}) = a_1 + a_2 q^{-1} + \ldots + a_{n_A} q^{-n_A+1} \tag{4.11}$$

$$\sum_{i=1}^{n_B} b_i q^{-i} = B(q^{-1}) = q^{-1}B^*(q^{-1}) \tag{4.12}$$

where: $B(q^{-1}) = b_1 q^{-1} + b_2 q^{-2} + \ldots + b_{n_B} q^{-n_B}$ (4.13)

$$B^*(q^{-1}) = b_1 + b_2 q^{-1} + \ldots + b_{n_B} q^{-n_B+1} \tag{4.14}$$

the model can be rewritten as:

$$y(t+1) = -A^* y(t) + q^{-d} B^* u(t) = -A^* y(t) + B^* u(t-d) \tag{4.15}$$

which can be expressed in the "linear regression" form given by:

$$y(t+1) = \theta^T \phi(t) \tag{4.16}$$

where $\theta^T = [a_1,...,a_{n_A},b_1,...,b_{n_B}]$ defines the vector of model parameters and $\phi^T(t)$ (also called "*regressor*") defines the vector of measurements and manipulated variables:

$$\phi^T(t) = [-y(t),..., y(t - n_A + 1), u(t - d),..., u(t - d - n_B + 1)] \tag{4.17}$$

Recursive Least Squares (RLS)

The essence of each adaptation scheme is given by the *parameter adaptation algorithm* (PAA) that is used to adapt the parameters of the predictor of the plant output.

For indirect adaptive control the goal of the PAA is to estimate as closely as possible θ, given $y(t+1)$ and $\phi(t)$ at each sampling time. Each PAA is derived with the objective of minimizing a criterion on the error between the plant and the model.

The parameter adaptation algorithms have a recursive structure, i.e. new estimated parameters can be obtained from the previous estimate plus a correction term which depends on the most recent measurements:

$$\begin{bmatrix}\text{New estimated}\\ \text{parameters}\\ (vector)\end{bmatrix} = \begin{bmatrix}\text{Previous estimated}\\ \text{parameters}\\ (vector)\end{bmatrix} + \begin{bmatrix}\text{Adaptation}\\ \text{gain}\\ (matrix)\end{bmatrix} \times \begin{bmatrix}\\ \text{Measurements}\\ (vector)\end{bmatrix} \times \begin{bmatrix}\text{Prediction}\\ \text{error}\\ (scalar)\end{bmatrix}$$

which can be expressed as:

$$\hat{\theta}(t+1) = \hat{\theta}(t) + F(t)\phi(t)\varepsilon(t+1) \tag{4.18}$$

For the Recursive Least Squares (RLS) *parameter adaptation algorithm*, the objective is to minimize the following criterion:

$$\sum_{i=1}^{t} \lambda_1^{(t-i)} \varepsilon^2(i-1) \tag{4.19}$$

Differently from other PAA, this approach guarantees a higher adaptation gain at the beginning (when the estimates are far from the true values) and a lower gain when $\hat{\theta}(t)$ is close enough to θ.

This approach leads to the following equations:

$$\varepsilon(t+1) = \frac{\varepsilon^0(t)}{1+\phi^T(t)F(t)\phi(t)} = \frac{y(t+1)-\hat{\theta}^T(t)\phi(t)}{1+\phi^T(t)F(t)\phi(t)} \tag{4.20}$$

$$\hat{\theta}(t+1) = \hat{\theta}(t) + F(t)\phi(t)\varepsilon(t+1) \tag{4.21}$$

$$F(t+1)^{-1} = F(t)^{-1} + \phi(t)\phi^T(t) \tag{4.22}$$

$$F(t+1) = F(t) - \frac{F(t)\phi(t)\phi^T(t)F(t)}{1+\phi^T(t)F(t)\phi(t)} \tag{4.23}$$

Initialization

Different initializations for this algorithm are possible, but the most common one is to assign an initial value for the adaptation gain in the form:

$$F(0) = \frac{1}{\alpha} I \text{ where } 0 < \alpha \ll 1 \tag{4.24}$$

This guarantees a high adaptation gain at the beginning of the process, when generally the initial estimate is not close to true values or it is even set arbitrarily. Typical values for α ranges from 0.001 to 0.1 depending on the precision of the first estimate.

4.2.2 Choice of the adaptation gain

The methodology described above is well suited only for stationary systems, i.e. when θ is not a function of time. If this is not the case, different variations of the algorithm are possible depending on the situation. All these modifications are based on a slightly different equation for $F(t+1)^{-1}$:

$$F(t+1)^{-1} = \lambda_1(t)F(t)^{-1} + \lambda_2(t)\phi(t)\phi^T(t) \tag{4.25}$$

$$0 < \lambda_1(t) \leq 1 \; ; \; 0 \leq \lambda_2(t) < 1 \; ; \; F(0) > 0$$

Note that $\lambda_1(t)$ and $\lambda_2(t)$ have opposite effects: $\lambda_1(t) < 1$ tends to increase the adaptation gain since more importance is accorded to new measurements, while $\lambda_2(t) < 1$ tends to decrease the adaptation gain, since lower importance is assigned to more recent measurements. The adaptation gain is modified in the following form:

$$F(t+1) = \frac{1}{\lambda_1(t)}\left[F(t) - \frac{F(t)\phi(t)\phi^T(t)F(t)}{\frac{\lambda_1(t)}{\lambda_2(t)} + \phi^T(t)F(t)\phi(t)}\right] \tag{4.26}$$

It is important to point out that different choices of $\lambda_1(t)$ and $\lambda_2(t)$ yield different PAA corresponding to different interpretations of the error criterion to be minimized.

Decreasing (vanishing) gain (RLS):

This is the standard form where:

$\lambda_1(t) = \lambda_1 = 1; \quad \lambda_2(t) = \lambda_2 = 1$

The error to be minimized is the one stated above; this form of PAA is well suited for time invariant systems since adaptation gain tends to decrease.

Constant forgetting factor:

In this case: $\lambda_1(t) = \lambda_1$; $0 < \lambda_1 < 1$; $\lambda_2(t) = \lambda_2 = 1$

This corresponds to the following error criterion to be minimized:

$$\min_{\hat{\theta}(t)} J(t) = \sum_{i=1}^{t} \lambda_1^{(t-i)} \left[y(i) - \hat{y}(i) \right]^2 \qquad (4.27)$$

This choice for $\lambda_1(t)$ and $\lambda_2(t)$ guarantees a lower weighting on old data; this explains the denomination of λ_1 as forgetting factor. Typical values for λ_1 range from 0.95 to 0.99. This form of RLS is well suited for systems with time-varying parameters.

Since the two-phase reactor considered presents time-varying parameters to be adapted, the last approach (constant forgetting factor) was selected for the adaptation of the model used by the MPC controller.

In Landau *et al.* (1998) many other possibilities are presented; these respond to much more precise demands and will be not covered here since they are not relevant for this work.

4.3 Single-Input Single-Output Model Weighting Adaptation on the two-phase reactor

As stated above, the first attempt will be conducted on the transfer function between u_2 and pressure (P). This is a logic decision since P/u_2 is the most troublesome

transfer fucntion due to its gain sign inversion. Note that this approach will be referred to as SISO MWA, because its goal is to adapt g_{P2} only.

Physically the gain sign inversion is explainable by the bi-molecular rate law: if species A is in excess in the gas phase, an increase in pure A feed will cause an increase in pressure; on the contrary if A is the limiting reactant, an increase in Feed 2 will allow a higher production (and consequently a higher consumption of C) that will cause a decrease in pressure.

Nevertheless, pressure doesn't depend only on pure A feed, so it is necessary to isolate the effect of Feed 2 only (u_2). Pressure dynamics can be seen as the sum of the contribution of the four manipulated variables:

$$P' = g_{P,1}u_1' + g_{P,2}u_2' + g_{P,3}u_3' + g_{P,4}u_4' \tag{4.28}$$

where:

- P' is Pressure in deviation variables (steady-state value of 2700kPa)
- u_i' is the i-th manipulated variable (deviation variables)

Since the effect on pressure of u_2 only is to be isolated, it was decided to substract the contribution given by the other manipulated variables, that is:

$$P_2' = P' - g_{P,1}u_1' - g_{P,3}u_3' = g_{P,2}u_2' \tag{4.29}$$

Note that the contribution given by u_4 (liquid inventoy setpoint) can be easily neglected since its effect is very small.

Since no information on g_{P1} and on g_{P2} is available, they were considered fixed and equal to the nominal case. This can be seen in fhe following figure:

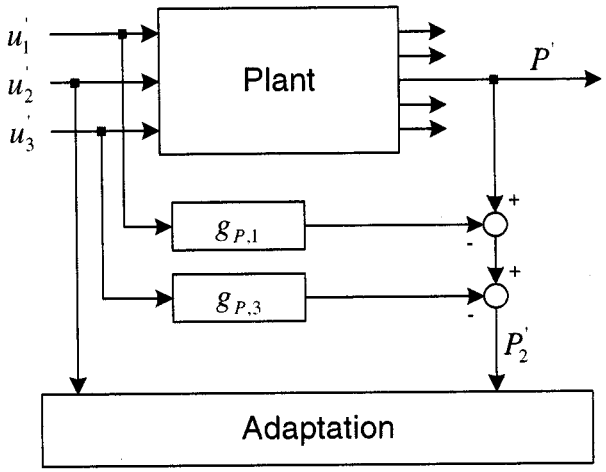

Figure 4.3: Isolation of u_2 effect on Pressure

The assumption of fixed g_{P1} and g_{P3} will prove to have a negative influence on the quality of information gathered by the adaptation algorithm. Nevertheless this choice represents a easy starting point to implement adaptation schemes.

4.3.1 Open-loop tests for the SISO MWA algorithm

The above described procedure was implemented on the plant in order to test MWA ability to identify a proper model for P_2/u_2 transfer function. In order to do so, model updating loop was not closed at this stage and consequently MWA was used as a pure identification tool. Furthermore, it was desired to test the extent to which isolation of Feed 2 (u_2) contribution is possible.

In the following analysis the focus is on the identified gains, rather than the resulting model including delays. This is reasonable since delays are negligible if compared to the system time constant.
Note that in MWA algorithm a delay range was included in order to give the algorithm more flexibility in treating undermodelling errors.

Gain range was fixed at [-60; 60] with a spacing of 5 and delay range was chosen equal to [0; 2] with a spacing of 0.2 hours. The resulting family is composed of 275 models. Time constant was fixed at 16 hours, consistently with the identification performed for MPC. Tests run at different conditions showed that g_{P2} characteristic time doesn't present large variations.

An 'initialization' of the algorithm was necessary before simulating the actual scenarios. In order to do this, a series of small setpoint changes on pressure (±10 kPa) were applied around nominal operating point. This allows the algorithm to have an estimate of g_{P2} at base case. The result of this operation was an identified gain close to reality; this inability to obtain the true gain at base case is indicative of the problems that will be encountered during actual scenarios.

In the following table a comparison between identified and true[3] gains is presented. The values shown are relative to the operating point corresponding to the end of each scenario.
For obvious reasons a more meaningful measure of the success of the identification performed is given by the comparison between time evolution of the true and identified K_{P2}. On the other hand, time evolution of true K_{P2} is not easily accessible, while steady-state gains can be easily obtained experimentally. Nevertheless, the trajectories followed by identified K_{P2} are presented in the Appendix.

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[3] True gains were obtained by means of step tests of ±1% on the manipulated variables

Table 4.1: Comparison between true and identified g_{P2} gains (K_{P2})

	Identified K_{P2}	True K_{P2}	W
Base Case	-30	-44	14.43
Scenario 1	-1.14	-37.08	14.11
Scenario 2	-18.7	-2.91	14.42
Scenario 3	9.8	0	11.3
Scenario 4	20	-14.56	15.92
Scenario 5	-14.3	27.44	15.64
Scenario 6	-9.4	-15.99	16.44

Before comparing true and identified g_{P2} gains (K_{P2}), it is important to discuss a few considerations concerning the weight map flatness (W). It is evident that values for W are relatively high if compared to $W_{\max} = \sqrt{N} = 16.58$, meaning that it is not possible to represent P/u_2 transfer function as the combination of few members of the model family.

Nevertheless, it must be noted that at the end of most scenarios (50 or 100 hours) W is still decreasing, implying that a better discrimination of model family members can be achieved. Furthermore, the flatness achieved with the SISO MWA approach can be considered as acceptable if compared to what will be obtained with the approach presented further in this chapter. Details about the profiles followed by weights, γ_i and W can be found in the Appendix.

The comparison of true and identified gains makes it clear that SISO MWA algorithm is not able to identify a proper model for g_{P2}. It is easily understandable that the use of fixed g_{P1} and g_{P3} may bias the data fed to the adaptation algorithm, leading to improper gain identification. In order to verify this, a comparison between nominal and

true g_{P1} and g_{P3} gains (which will be refered to as K_{P1} and K_{P3}) is necessary for the different scenarios. This comparison is presented in the following table.

Table 4.2: g_{P1} and g_{P3} gains for the different scenarios

	K_{P1}	K_{P3}
Base Case	47.96	-10.42
Scenario 1	93.98	-9.44
Scenario 2	27.86	-5.43
Scenario 3	41.15	-8.54
Scenario 4	47.94	-2.86
Scenario 5	27.75	-30.45
Scenario 6	37.31	-5.02

Table 4.2 clarifies the reasons why the proposed procedure leads to improper identification for g_{P2}: K_{P1} and K_{P3} change substantially during the different scenarios, and consequently the use of fixed constant g_{P1} and g_{P3} (to isolate u_2 contribution) introduces a large error. This error is in the form of over- or under-estimation of contribution given by u_1 and u_3 and leads to an improper identification of K_{P2} in order to compensate error on K_{P1} and K_{P3}.

Given the large variations of K_{P1} and K_{P3} observed it is not surprising that the SISO MWA approach does not provide proper model identification. The most logical solution to this problem will be the attempt to adapt g_{P1}, g_{P2} and g_{P3} at the same time, as shown later in this chapter.

In order to better understand the identification problems encountered, it is also important to point out that most of the scenarios tested (4 out of 6) result from a

disturbance entering the system. This makes the success of adaptation techniques even more challenging since information fed to the adaptation scheme may not be as rich as in the case of set point changes.

It is also important to note that at this stage no excitation signal was added and the identification scheme has to rely only on the process-generated disturbances that generally provide little information. This obviously has a negative impact on the quality of the identification obtained and further attempts should be carried out in this direction.

It may also be argued that problems arise also because the system is not well suited for the MWA scheme. In order to verify this, a Recursive Least Square (RLS) approach was also used and the results found confirmed to a certain extent what was observed for the MWA algorithm. Details can be found later in this chapter.

4.3.2 Results for the closed-loop SISO MWA

Despite the identification problems encountered, the above described adaptation scheme was implemented with the 'adaptation' loop closed. Consequently the new model estimate obatained through the MWA algorithm is used to update the model incorporated in the MPC controller. Obviously only P/u_2 transfer function was updated.

Plant model is estimated at each sampling time (0.1 hours), while model updating can be performed at each sampling time, or less frequently. It was decided to update MPC model every 10 sampling times, (i.e. every hour). This choice represents a trade-off between the need to use the most recent (and theoretically the most accurate) estimate obtained and the need to 'filter' the model used by MPC. This latter aspect can be more

easily understood observing the profile of estimated K_{P2}, that in some cases show quick and large variations (see the Appendix).
Results obtained from the closed-loop implementation of MWA are shown and discussed in section 4.4.3 together with the results obtained through the multivariable approach.

4.3.3 Concluding remarks

In the last sections a single-input single-output MWA algorithm was used in order to adapt g_{P2} transfer function. Identification problems arose during the preliminary test on the open-loop algorithm and the reason for these problems was identified in the assumption of fixed and constant g_{P1} and g_{P3}. The problems encountered suggested the need to compare the results found with a different adaptation algorithm, as it will be discussed further in this chapter. Also, another possible approach is represented by a multivariable adaptation of g_{P1}, g_{P2} and g_{P3}, as it is discussed in the following sections.

Despite the problems encountered, it was decided to test MWA algorithm in closed-loop. The results are shown in section 4.4.3. The performance observed was comparable to that obtained with the fixed-model MPC discussed previously. In some cases a slight improvement was observed but generally speaking more oscillatory behaviour was encountered.

4.4 Multivariable Model Weighting Adaptation on the two-phase reactor

In the last sections an attempt was made to reduce model mismatch when operating conditions change. The selected approach was model weighting adaptation on P/u_2 transfer function. Problems were encountered in isolating the contribution given by u_2 and consequently improper gain identifications resulted. The main reason for this failure was identified in the use of fixed gains for g_{P1} and g_{P3}.

The natural solution to this problem is to extend the adaptation to transfer functions g_{P1} and g_{P3}. This leads to a multi-input single-output (MISO) MWA algorithm. Once again, the effect given by u_4 is neglected for the same reasons as above.

4.4.1 Extension of the MWA algorithm to the MISO case

The algorithm presented in section 4.1 is the same as in Gendron (1998) and it is developed for a SISO process. The extension to the MISO case is very straightforward, but it is still worth briefly discussing the main differences.

In section 4.3 pressure dynamics had been considered as the sum of the effects given by manipulated variable u_1, u_2 and u_3 (u_4 contribution was neglected), expressed in the following form:

$$P' = g_{P,1}u_1' + g_{P,2}u_2' + g_{P,3}u_3' \qquad (4.30)$$

Since it was not possible to identify only g_{P2}, we now try to identify g_{P1}, g_{P2} and g_{P3} simultaneously. This implies that not only one, but three model families have to be specified. Furthermore, error can be calculated with respect to the sum of the three contributions. This implies that a weight must be assigned for each possible combination of models, which means $N_1 \cdot N_2 \cdot N_3$ combinations (where N_i is the number of models belonging to the i-th family).

Weights are assigned in the same way as in the SISO case. For model $P_{i,j,k}$ (corresponding to the combination of models $P_{1,i}$, $P_{2,j}$ and $P_{3,k}$) truncated 2-norm of error is calculated by:

$$\left\| e_{i,j,k}(t) \right\|_{2,\lambda}^2 = \sum_{k=0}^{t} \lambda^{t-k} e_{i,j,k}^2(k) \tag{4.31}$$

with:

$$e_{i,j,k}(k) = P'(k) - P_{1i}'(k) - P_{2j}'(k) - P_{3k}'(k) \tag{4.32}$$

where, for example, $P_{1i}'(k)$ is u_1 contribution on pressure predicted by the i-th model of the first model family. It is important to recognize that the way of numbering family members here is different since it uses only one index (i.e. i goes from 1 to N_1, number of models on F_1).

Weight to be assigned to model $P_{i,j,k}$ can be easily calculated by:

$$w_{i,j,k}(t) = \frac{\left(\mu + \left\|e_{i,j,k}(t)\right\|_{2,\lambda}^{2}\right)^{-1}}{\sum_{\text{mod } els}\left(\mu + \left\|e_{i,j,k}(t)\right\|_{2,\lambda}^{2}\right)^{-1}} \tag{4.33}$$

Once again, the small positive constant μ is introduced to prevent any possible division by zero.

The resulting models for $g_{P,1}$, $g_{P,2}$ and $g_{P,3}$ (named $\hat{g}_{P,1}$ $\hat{g}_{P,2}$ and $\hat{g}_{P,3}$) can be easily computed from the weights assigned to each possible combination. First a 'partial' weight (δ) for each member of F_1, F_2 and F_3 is calculated, and then the resulting model is built as it was for the SISO case. For example, for the first model family:

$$\delta_{1,i} = \sum_{j=1}^{N_2}\sum_{k=1}^{N_3} w_{i,j,k} \qquad \text{with } i = 1,2...N_1 \tag{4.34}$$

$$\gamma_{1,1} = \sum_{i=1}^{L_{g1}} \delta_{1,i} g_{1,i}\ , \quad \gamma_{1,2} = \sum_{i=L_{g1}+1}^{2L_{g1}} \delta_{1,i} g_{1,i}\ , \quad \gamma_{1,3} = \sum_{i=2L_{g1}+1}^{3L_{g1}} \delta_{1,i} g_{1,i}\ \ldots. \tag{4.35}$$

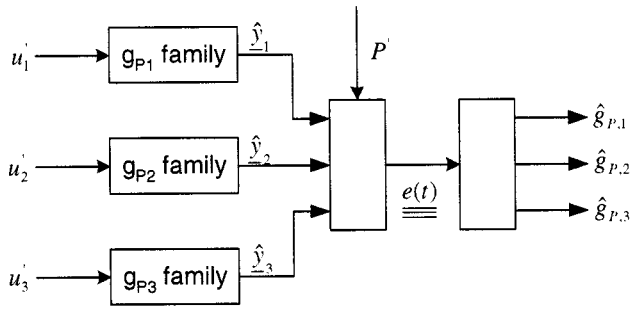
The resulting model given by F_1 is:

$$\hat{g}_{P,1}(z^{-1}) = \frac{1-\alpha_1}{1-\alpha_1 z^{-1}} \sum_{j=1}^{L_{d1}} \gamma_{1,j} z^{-d_{1,j}-1} \tag{4.36}$$

Where $L_{g1} = card(G_1)$ and $L_{d1} = card(D_1)$, with G_1 and D_1 the sets of possible gains and delays for the first model family.

It is easily understandable that, if gain and delay ranges are not selected properly, a huge number of possible combinations can be easily obtained.

The algorithm described for MISO MWA can be viewed in the following flowsheet:



4.4.2 Open-loop tests for the MISO MWA algorithm

The above described procedure was implemented on the reactor to test MWA ability to properly estimate models for g_{P1}, g_{P2} and g_{P3}. Similarly to what done for the SISO case, at this stage the model update loop was not closed, using MWA as a pure identification tool. The process is controlled by the MIMO MPC discussed in Chapter 3.

As explained previously, prior to implementing MWA, gain and delay ranges have to be fixed for each model family. Gain ranges were chosen following step test performed at different operating conditions. Delay ranges were introduced for g_{P1} and g_{P3} in order to take into account minor deviations from first-order dynamics. For example, at nominal point g_{P2} presents a minor inverse response wich can be approximated by a delay. See the Appendix for details.

Finally gain and delay ranges were chosen as follows:

$G_1 = [20,30,...,60]$; $D_1 = [0]$

$G_2 = [-50,-30,...,50]$; $D_2 = [0,1,2]$

$G_3 = [-35,-30,...,-5]$; $D_3 = [0,1,2]$

Before running the actual scenarios, it is necessary to 'initialize' the algorithm. This must be done so that MWA has an initial estimate of the plant. The initialization is done by applying a series of small steps on pressure setpoint (± 10 kPa); setpoints are filtered in order to have a first-order reference trajectory ($\tau = 2.4$ hours). This procedure finally constitutes a system identification around the nominal operating point, and the results obtained can be seen as a first measure of the precision obtainable with the MISO MWA approach. Gain estimates for g_{P1}, g_{P2} and g_{P3} around base case are shown in Table 4.3.

Starting from this initial estimate of the plant, MWA algorithm (with no model updating) was tested during the 6 scenarios described in section 2.2.2. The following tables show a comparison between identified and true gains for g_{P1}, g_{P2} and g_{P3} at the operating points corresponding to the end of each scenario. Weight map flatness (W) is also shown for each case.

Once again, it would be more meaningful to compare the time evolution of the true and identified gains; this comparison was not performed due to the difficulties in obtaining time evolutions of the true gains. Nevertheless trajectories followed by identified K_{P1}, K_{P2} and K_{P3} are presented in the Appendix.

Table 4.3: Gains identified by the multivariable MWA

	Identified K_{P1}	Identified K_{P2}	Identified K_{P3}	W
Base Case	39.97	-1.74	-13.75	31.33
Scenario 1	39.75	-1.02	-18.51	31.71
Scenario 2	38.95	-1.72	-18.65	32.14
Scenario 3	40.15	12.92	-19.69	29.66
Scenario 4	37.29	8.69	-16.28	31.99
Scenario 5	31.18	-6.09	-18.39	32.39
Scenario 6	41.47	-6.88	-10.33	29.10

Table 4.4: True gains of g_{P1}, g_{P2} and g_{P3}

	True K_{P1}	True K_{P2}	True K_{P3}
Base Case	47.96	-44.29	-10.42
Scenario 1	93.98	-37.08	-9.44
Scenario 2	27.86	-2.91	-5.43
Scenario 3	41.15	0	-8.54
Scenario 4	47.94	-14.56	-2.86
Scenario 5	27.75	27.44	-30.45
Scenario 6	37.31	-15.99	-5.02

Looking at Table 4.3 and Table 4.4, it is evident that identified and true gains are far from each other. In particular it can be observed that identified gains are always very close to the average of the range specified for each family (40, 0 and -20 respectively). This suggests that in this case MWA algorithm is not able to discriminate between the different possible models belonging the the families and the resulting model is very close to the average model (i.e. the one obtained with uniform weights). This is

confirmed by the high values of W, which are always very close to $W_{\max} = \sqrt{N_1 \cdot N_2 \cdot N_3} = 32.86$, corresponding to the uniform weight map.

Different reasons for this failure were identified. These reasons are outlined here but no detailed explanation will be given, since no extensive study was carried out on this aspect.

1. A problematic aspect of this application is given by the very similar time constant characterizing g_{P1}, g_{P2} and g_{P3}. Model families F_2 and F_3 have a time constant $\tau = 16$ while F_1 was built with $\tau = 15$.

2. Gain ranges presented by transfer functions contributing to pressure dynamics probably represent the most troublesome aspect of this process. It is important to point out that $G_2 = [-60;60]$ has an overlap with both G_1 and G_3. This makes it very difficult, if not impossible, to assign the contribution given by each transfer function to the total pressure dynamics.

3. Implementation of the MISO MWA approach is complicated even more by the fact that in real scenarios MVs are moved at the same time. This makes it almost impossible to isolate the separate contribution of g_{P1}, g_{P2} and g_{P3} to pressure variation. It was tested on a linear model of the plant that if inputs are moved sequentially, even with short delays between the moves of different variables, $\hat{g}_{Pi}$ (with $i=1,2,3$) quickly reaches a reasonable estimate of g_{Pi}.

4. At this stage, no excitation signal was used and the algorithm must rely only on the process-generated information. Obviously, this aspect limts the quality of the identification obtainable.

4.4.3 Results for the closed-loop MISO MWA

Up to this point MWA was used as a pure identification tool since the model known by the controller was not updated with the new information obtained through the MWA algorithm. Despite the identification problems encountered with the MISO MWA approach, the system was tested with the adaptation loop closed.

As for the SISO MWA strategy, it was decided to update the model known by the MPC controller at every 10 sampling times (i.e. every hour). Once again this represents a trade off between using the latest (and theoretically the most accurate) estimate obtained, and the need to filter the model fed to the MPC. In fact, during transient conditions, estimated gains present quick and large variations as can be seen in the Appendix.

Here results from both the SISO MWAC strategy and the MISO MWAC strategy are discussed. The explanation of certain behaviours remains somehow obscure and would require a more detailed analysis, but nevertheless it is important to point out some important considerations.

In Figure 4.4 and Figure 4.5 results from scenario 1 (disturbance in feed composition) are presented. In this case SISO MWAC gives performance comparable, if not better than MPC with fixed model. The SISO MWAC approach gives a trajectory for y_{A3} very close to the one obtained with the standard MPC strayegy, while pressure and product flow trajectories show some improvement.
This improvement is possible since in this scenario u_2 is not used to control pressure, but only to correct the purge composition. Consequently, errors on esimated K_{P2} do not have significant consequences on the computed control sequence.

On the contrary, it is evident how the attempt to adapt g_{P1}, g_{P2} and g_{P3} negatively affects the global performance of the MPC controller. Even if production rate is kept within ± 5% of its nominal value and pressure doesn't go over its uper limit (i.e scenario objectives are achieved), the resulting performance is much lower than the one obtained with the fixed-model MPC.

It is interesting to note that in both cases y_{A3} trajectory is minimally affected by the adaptation schemes used. This minimal effect is because y_{A3} depends almost exclusively on Feed 2 (u_2) and that transfer function (y_{A3}/u_2) was not adapted. This happens not only for scenario 1 but for all the situations where the demanded setpoint is possible.

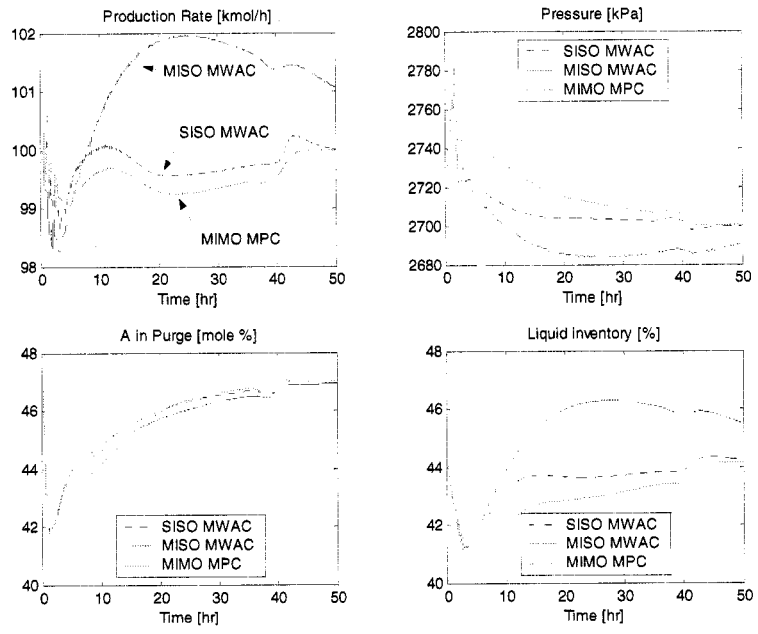


Figure 4.4: Scenario 1 – Controlled variables – SISO MWAC (dotted black), MISO MWAC (dashed blue) and MIMO MPC (solid green)

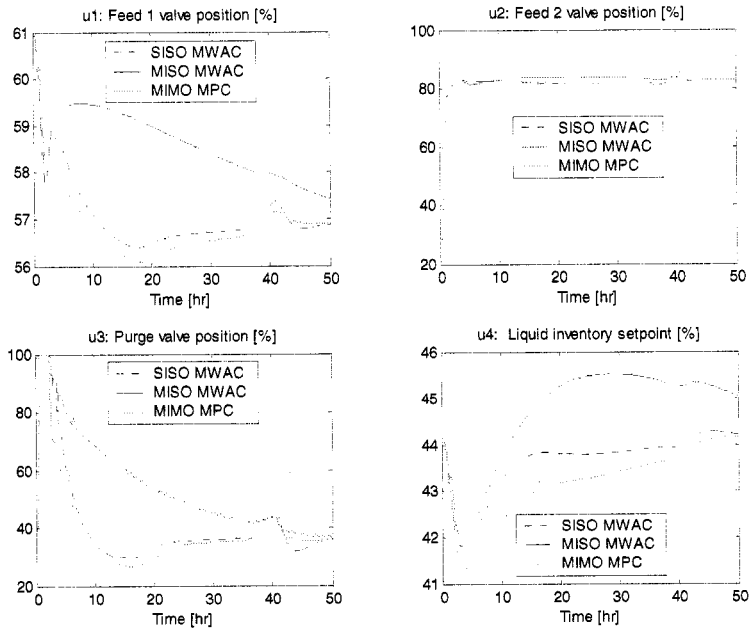


Figure 4.5: Scenario 1 – Manipulated variables – SISO MWAC (dotted black), MISO MWAC (dashed blue) and MIMO MPC (solid green)

In Figure 4.6 and Figure 4.7 results from scenario 2 (change in production setpoint) are presented. In this case results obtained with the three strategies are very similar. The adaptation of g_{P2} only (SISO MWAC approach) gives output trajectories almost identical to the fixed-model MPC, but some minor oscillations are introduced on pressure. This result is possible because pressure is not controlled by means of u_2. Also, the estimation of K_{P2} is closer to the true value than the nominal gain used for standard MPC.

The MISO MWAC approach still gives acceptable performance, but it is definitely less interesting than the previous approaches: production rate presents an overshoot and oscillations on pressure are more important due to oscillatry control actions on u_3.

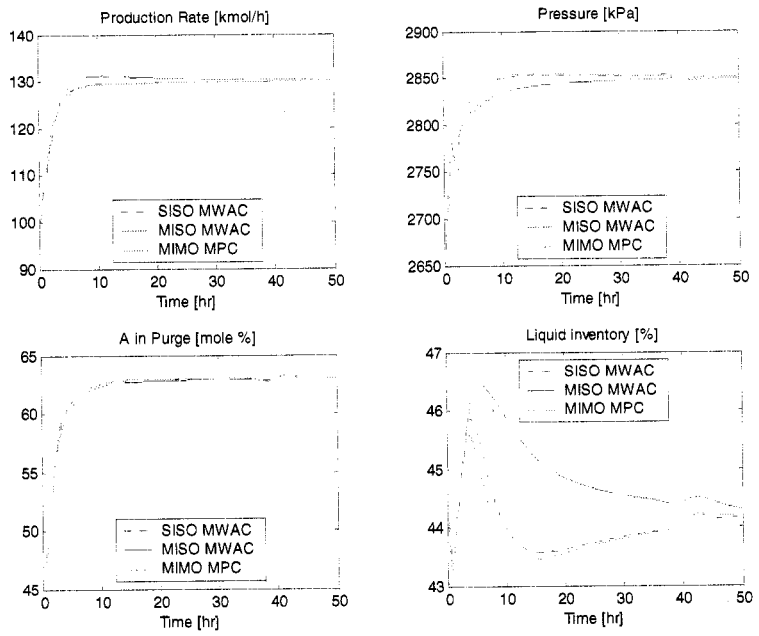


Figure 4.6: Scenario 2 – Controlled variables – SISO MWAC (dotted black), MISO MWAC (dashed blue) and MIMO MPC (solid green)

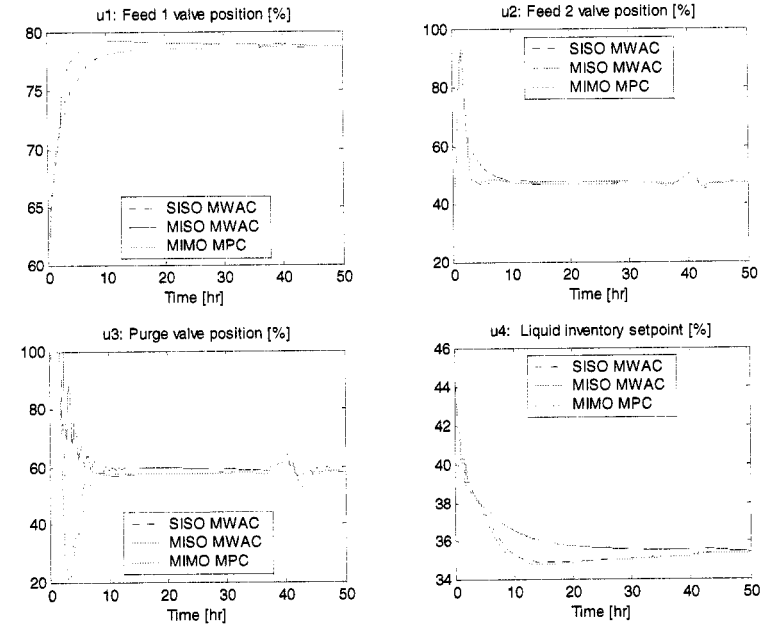


Figure 4.7: Scenario 2 – Manipulated variables – SISO MWAC (dotted black), MISO MWAC (dashed blue) and MIMO MPC (solid green)

As it was the case for scenario 2, also in the case of a sudden loss of F_2 (scenario 3), both adaptation strategies present results very similar to the MPC aproach. In this case there is a certain improvement for pressure trajectory, but this is obtained at the cost of a faster decrease in production rate. Once again some oscillations are present on pressure trajectory, but in this case they are less important.

It is important to note that both adaptation approaches move u_1 differently from the fixed-model MPC. This difference is because, for different reasons, K_{P2} is identified as close to zero (true value) and consequently u_2 is not used to control pressure. This fact implies that as soon as u_3 saturates, u_1 is quickly decreased in order to limit pressure increase. On the contrary, MIMO MPC strategy waits for u_2 saturation before decreasing the main feed to the reactor (u_1).

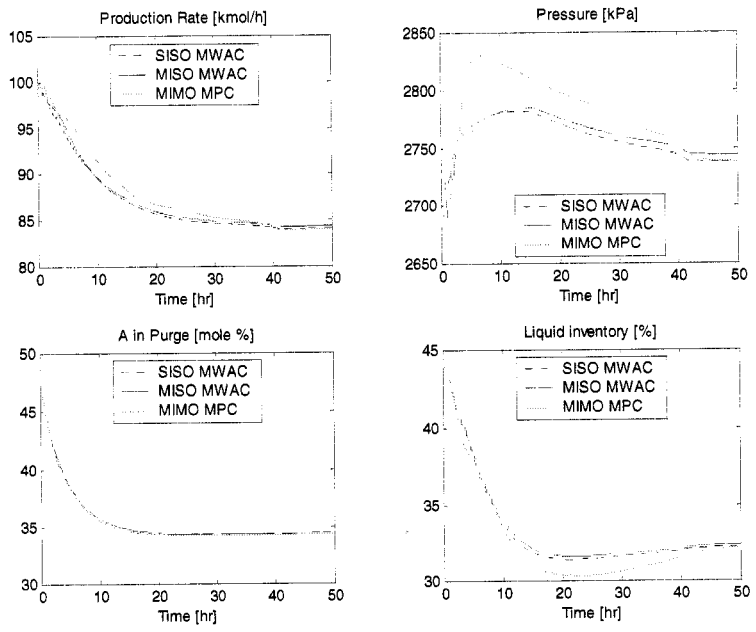


Figure 4.8: Scenario 3 – Controlled variables – SISO MWAC (dotted black), MISO MWAC (dashed blue) and MIMO MPC (solid green)

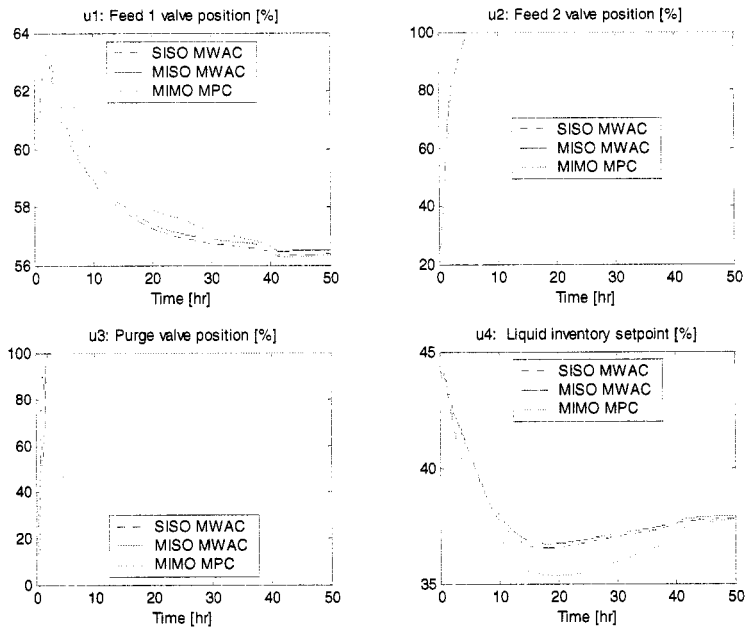


Figure 4.9: Scenario 3 – Manipulated variables – SISO MWAC (dotted black), MISO MWAC (dashed blue) and MIMO MPC (solid green)

In Figure 4.8 and Figure 4.9 results in the case of a drift in kinetic parameters (scenario 4) are shown. Similarly to the preceding scenario, the starting operating point is no longer possible and a certain degree of freedom is left to the controller to determine the resulting operating point. This is calculated according to the weights assigned and the model known by the controller. In this sense, model adaptation explains the different operating points obtained.

On the other hand, the patterns of response are very similar for the three approaches and no particular problem is encountered. This is possible since this scenario doesn't require a fast control action, but rather a slow and steady shift of the operating point.

It is important to point out that in the fixed-model MPC approach y_{A3} was *'sacrificed'* in order to decrease pressure by means of manipulating u_2, because of the negative gain *known* by the controller. On the contrary, both adaptation schemes lead to the

inacccurate identification of a positive gain for g_{P2}, which leads to the choice of decreasing u_2 in order to keep y_{A3} close to its setpoint and reduce pressure at the same time. The effect on pressure is opposite to the expected one (note that the true g_{P2} gain is negative) and this results in the need to decrease Feed 1 (u_1) in order to satisfy the shutdown-limit.

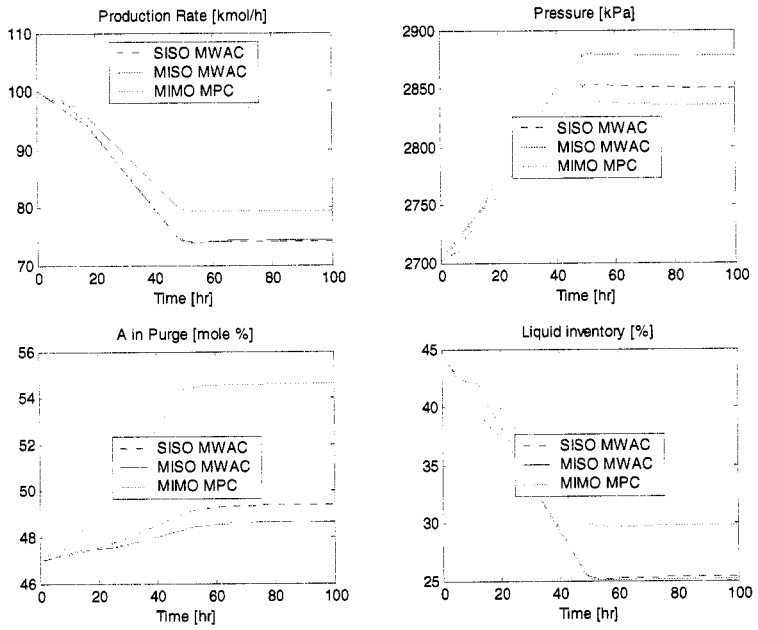


Figure 4.10: Scenario 4 – Controlled variables – SISO MWAC (dotted black), MISO MWAC (dashed blue) and MIMO MPC (solid green)

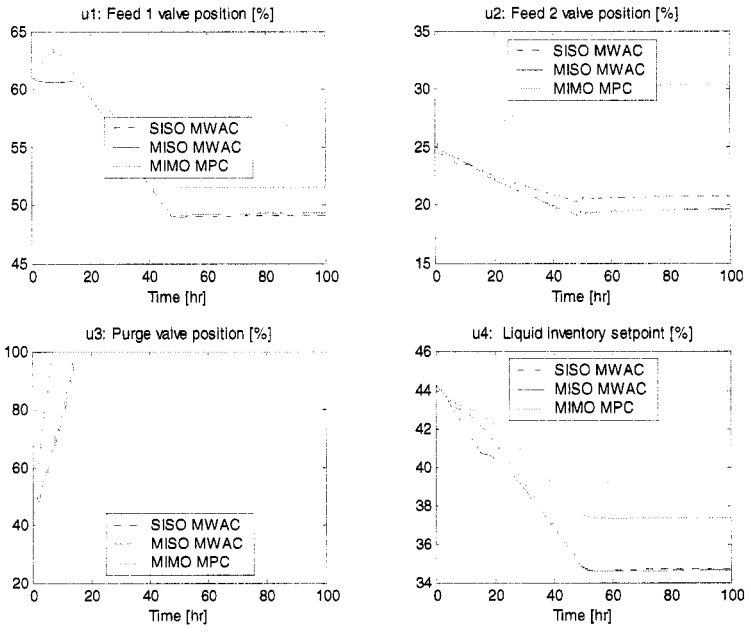


Figure 4.11: Scenario 4 – Manipulated variables – SISO MWAC (dotted black), MISO MWAC (dashed blue) and MIMO MPC (solid green)

In Figure 4.12 and Figure 4.13 results from scenario 5 are presented. In this case a setpoint change on y_{A3} is demanded while requiring other outputs to remain at the nominal value. This scenario presents a gain sign inversion of g_{P2}, and the introduction of adaptation techniques was expected to have positive influence on performance. Nevertheless, the inability to properly identify g_{P2} gain prevents this improvement and a performance deterioration was observed.

As was the case for most scenarios, no significant differences are observed on composition dynamics. On the contrary, pressure and product flow trajectories show a decrease in performance. The reasons for this effect are not clear but certainly the quick changes in estimated gains, together with the imprecise gains used, are key elements.

It is important to recognize that performance obtained with both adaptation schemes is still acceptable, but the improvement expected was not obtained and fixed-model MPC proved to be better suited to ths problem.

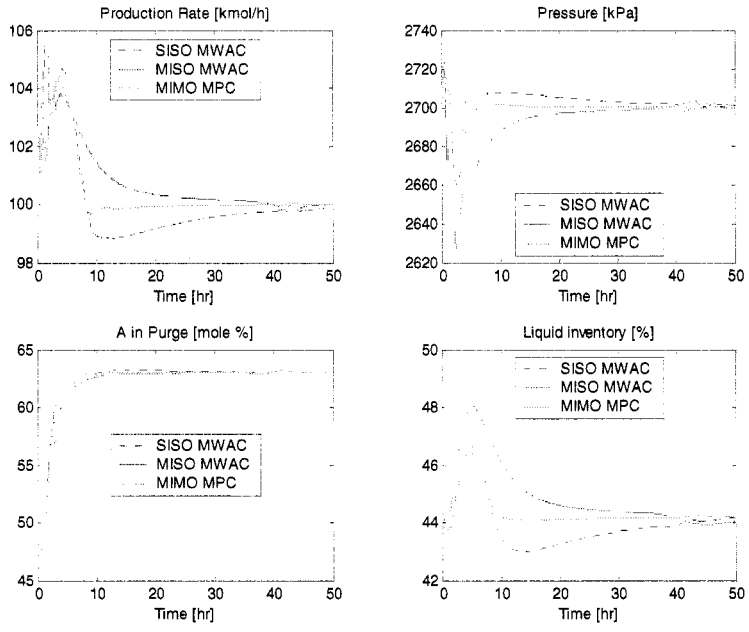


Figure 4.12: Scenario 5 – Controlled variables – SISO MWAC (dotted black), MISO MWAC (dashed blue) and MIMO MPC (solid green)

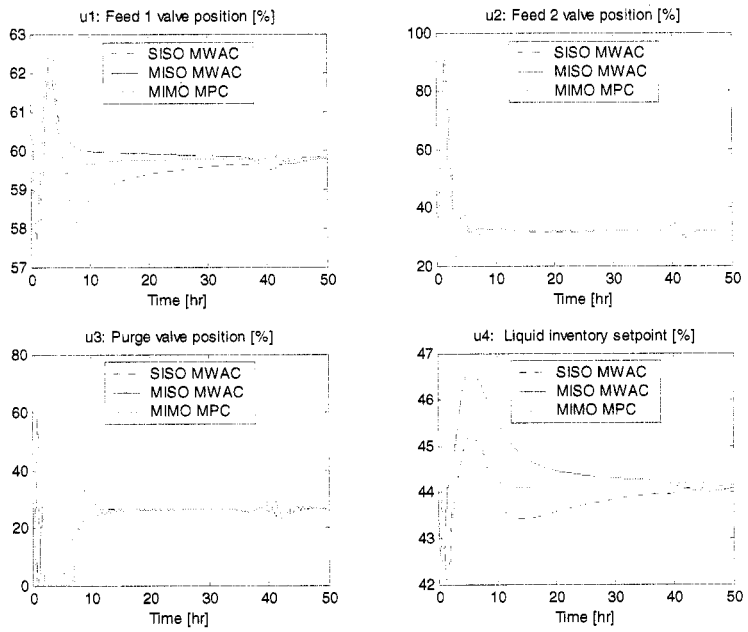


Figure 4.13: Scenario 5 – Manipulated variables – SISO MWAC (dotted black), MISO MWAC (dashed blue) and MIMO MPC (solid green)

In the following figures results from scenario 6 are presented. In this low demanding scenario SISO MWAC approach gives results very similar to the fixed-model MPC. This is possible since g_{P2} is not very important in determining optimal control moves. In fact, u_3 has sufficient authority to control pressure (no valve saturation is encountered) and thus u_2 is not used in this sense, but only to correct purge composition. Furthermore u_2 is not largely moved, so the influence of errors on g_{P2} is not very important.

On the other hand, if a MISO MWA aproach is used, a substantial decrease in performance is observed. This is in the form of larger deviation from setpoint and oscillations. Oscillations on pressure are due to the quickly-changing identified K_{P3}, which determines 'corrections' on the manipulated variable trajectory.

The larger deviations from setpoint are due to the less aggressive trajectories followed by manipulated variables. The reasons for such differences are more obscure, but cerainly the higher model mismatch plays a role in this decrease of performance.
Deviation from setpoint is not high in magnitude, but it is 3-4 times larger than that obtained with the fixed-model MIMO MPC.

However, it is important to point out how both adaptation strategies give results comparable to the MIMO MPC approach: the same pattern of response is kept and deviations from setpoint are totally acceptable. The major problem resides in the oscillations encountered with the MISO MWAC strategy, which in some cases can be reduced by increasing the model updating frequency.

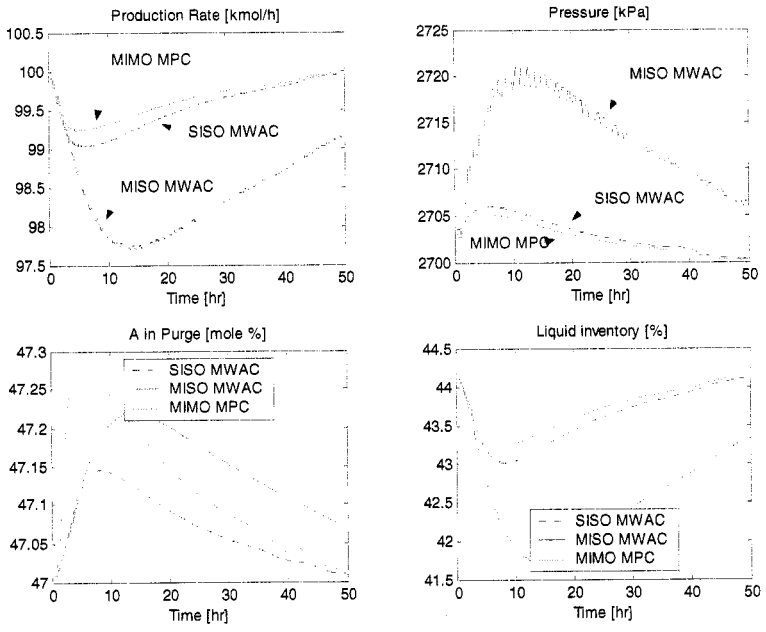


Figure 4.14: Scenario 6 – Controlled variables – SISO MWAC (dotted black), MISO MWAC (dashed blue) and MIMO MPC (solid green)

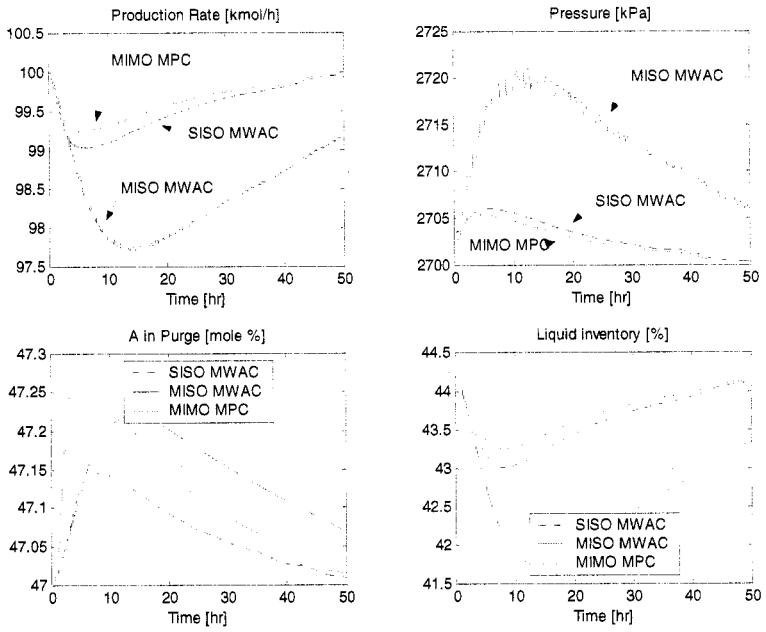


Figure 4.15: Scenario 6 – Manipulated variables – SISO MWAC (dotted black), MISO MWAC (dashed blue) and MIMO MPC (solid green)

4.4.4 Concluding Remarks

In the last sections, a multivariable MWA algorithm was used in the attempt of adapting pressure dynamic model (g_{P1}, g_{P2} and g_{P3} simultaneously) and serious identifiability problems were encountered. In particular, the algorithm wasn't able to discriminate among the family members and the resulting model was often the uniform combination of all family members.

Model adaptation loop was closed despite the problems encountered. As expected, the improper identification of g_{P1}, g_{P2} and g_{P3} negatively affected control performance and stability. The results found were acceptable, but no improvement was obtained

throught the adaptation techniques. In particular, oscillations and higher deviations from setpoint were observed.

Both SISO and MISO MWA approaches made it clear that the application considered (and particularly pressure dynamics) shows some serious identifiability issues. In the following sections another algorithm will be used but no particular improvement was encountered.

4.5 RLS approach on the two-phase reactor

In the previous sections MWA showed serious problems in identifying proper models for g_{P1}, g_{P2} and g_{P3}. In the SISO case the over/under-estimation of g_{P1} and g_{P3} gain was identified as the main cause for this failure. On the other hand, in the MISO case the algorithm wasn't able to discriminate between the family members and the resulting model for $\hat{g}_{P,i}$ corresponded to a uniform combination of family members.

In the following sections a classic Recursive Least Square algorithm will be tested on the system in order to validate the results obtained with the MWA approach. An overview of the algorithm used can be found in section 4.2 of this work and details are in Landau *et al.* (1998).

Note that, similarly to MWA approach, no excitation was added to the process-generated signals.

4.5.1 SISO approach

First, a SISO strategy was used to identify g_{P2} gain (K_{P2}). Transfer function g_{P2} is assumed to follow first-order dynamics with a fixed time constant $\tau = 16$ and gain determined by the RLS algorithm.

In order to isolate the effect of u_2 on the pressure dynamics, u_1 and u_3 contribution (according to the nominal model) were substracted to the total pressure variation (see Figure 4.3). Also, in this case g_{P1} and g_{P3} were assumed constant and this will prove to affect negatively the quality of the estimates obtained.

Once again, the algorithm was initialized through a series of small steps on pressure setpoint (± 10 kPa). This consitutes a plant identification around nominal operating point and thus, a first measure of the precision given by this approach for this application. This yielded an identified K_{P2} of -41.97, which is very close to the true value.

The following table presents a comparison between true gains and the gains identified by SIOS MWA and SISO RLS approaches.

Table 4.5: True and identified g_{P2} gains; MWA and RLS approaches

	Identified K_{P2} (RLS)	Identified K_{P2} (MWA)	True K_{P2}
Base Case	-41.97	-30	-44
Scenario 1	7.11	-1.14	-37.08
Scenario 2	-37.50	-18.7	-2.91
Scenario 3	-65.08	9.8	0
Scenario 4	23.85	20	-14.56
Scenario 5	-37.82	-14.3	27.44
Scenario 6	-34.22	-9.4	-15.99

Table 4.5 clearly shows that the proposed SISO RLS algorithm is not able to adequately identify the gain for g_{P2}, but this is not surprising. Nevertheless, it is interesting to comment on some considerations on the difference between the gains identified by MWA and RLS algorithms.

In most scenarios (all except scenario 3) both approaches show an error of the same sign. This fact represents a confirmation of the results obtained with the MWA algorithm and it is clearly due to the assumption of constant and fixed g_{P1} and g_{P3} that leads to an over/under-estimation of u_1 and u_3 contribution.

Differences in the values obtained are observable because the RLS algorithm is much slower than MWA in converging to a final estimate. This implies that that the rich input/output data fed to the algorithm does not last enough to obtain a final estimate. In order to overcome this problem an excitation signal should be added, but this would not improve the quality of adaptation during transient conditions.

The last consideration suggests that RLS is not suited for this application since its 'convergence time' is much longer than the closed-loop dynamic obtained with the multivariable MPC controller discussed in Chapter 3.

Nevertheless, it can be stated that the RLS approach discussed here validates to a certain extent the results obtained with the MWA algorithm, but problems were encountered.

4.5.2 MISO approach

A MISO approach was also tested in order to identify g_{P1}, g_{P2} and g_{P3} gains (K_{P1}, K_{P2} and K_{P3}); g_{P1}, g_{P2} and g_{P3} are assumed to follow first-order dynamics with fixed time constant and gain determined byt the RLS algorithm.
Similarly to the SISO RLS approach, the MISO RLS algorithm discussed in this section was tested with the adaptation loop open (i.e. the algorithm is used as a pure identification tool).

The identification of K_{P1}, K_{P2} and K_{P3} simultaneously proved to be an unrealistic goal for this approach. The factors determining the failure of the MISO MWA algorithm are not avoided with this algorithm and the consequences in this case are even more serious. In particular, since no gain ranges are provided, gain estimates are free to move to unreasonable values. These can be in the form of excessively large values or physically impossible signs (e.g. negative K_{P1} or positive K_{P3}).

The reasons for the failure of this approach are roughly the same as for the MWA algorithm: very similar time constant for the three transfer functions and the simultaneous manipulation of the MVs. Nevertheless, the latter factor plays a much more important role than before because of RLS slowness to converge to new estimates.

4.5.3 Concluding remarks

In the last sections an RLS technique was tested in order to validate the results found with the MWA algorithm. In both SISO and MISO approach, the adaptation loop was not closed, thus using the algorithm as a pure identification tool.

In most cases the SISO RLS gave results quite different from the corresponding MWA strategy. Nevertheless, it was shown how they partially confirm what was previously found. A mattern of concern is represented by the slow convergnece speed guaranteed by the RLS algorithm.

On the other hand, the MISO RLS approach proved to be unsuccessful. In particular, the unboundedness of identified gain results in unreasonable or physically impossible values. Once again RLS convergence speed was an issue.

It must be noted that the application considered shows serious identifiability problems regardless of the algorithm used. Clearly, this has negative consequences for the use of adaptation techniques. This is particularly true for pressure dynamics because of its truly multivariable nature and because of the gain ranges and time constants presented by the transfer functions involved.

CHAPTER 5 Conclusions and recommendations

5.1 Conclusions

The goal of this work was to improve the control performance and stability of the two-phase continuous reactor presented in Ricker (1993). The multivariable and constrained nature of the problem suggested the choice of an MPC algorithm. Changing conditions and process nonlinearities suggested the possibility of using model adaptation techniques. As stated in the introduction of this work, three strategies were developed and compared.

First, a mixed strategy was attempted. This consists of a standard multiloop strategy where the pressure loop is regulated by a monovariable MPC controller. This strategy resulted in a sensible performance improvement compared to the corresponding multiloop PI strategy discussed in Ricker (1993). However some limitations are caused by the use of a decentralized strategy and by valve saturation phenomena.

Next a multivariable MPC strategy was attempted in order to overcome some of the problems encountered with the previous approach. The resulting performance obtained is highly improved: reference trajectory is tracked very closely during setpoint changes and disturbances are rejected quickly and efficiently. The reasons for this success were identified in the multivariable approach and in MPC predictive behaviour. Nevertheless, some problems were encountered for tuning: in particular, weighting factors were not

dictated only by process and economic priority for each variable but also by stability considerations.

In order to overcome the limitations given by the use of a fixed model, adaptation techniques were attempted. The focus was set on the pressure dynamics because of its characteristic gain sign inversion and because of the constrained nature of this variable. The selected approach was Model Weighting Adaptation because of its simplicity and convergence speed.

First, a monovariable approach was attempted in order to update the model of the only transfer function presenting a gain sign inversion. Some identifiability problems were encountered, in particular due to the difficulty in isolating the contribution on pressure given by pure A Feed only. Consequently, a multivariable approach was attempted. This showed even more serious identifiability problems, resulting in the algorithm's inability to discriminate between model family members.

Despite the problems encountered, this algorithm was tested with the adaptation loop closed. For the monovariable approach closed-loop results were comparable, if not slightly better than the fixed-model MPC. On the other hand, problems encountered in the multivariable approach resulted in significant degradation of control performance, with the appearance of oscillations and a larger deviation from reference trajectory.

5.2 Recommendations

The following considerations have the aim of suggesting some possible improvements and indicating future research paths.

1. In certain scenarios it was observed that the original operating point was no longer possible. In these cases some freedom was left to the MIMO MPC in

determining the new operating conditions. The possibility of adding a supervisory layer to face these circumstances could be studied. This would have the goal of driving the system to the most desirable operating point (maximising production and/or minimizing operating costs).

2. The last chapter showed that this application shows identifiability problems with negative consequences on adaptation techniques. This aspect of the application could be studied in more detail in order to overcome some of the difficulties encountered.

3. The nonlinear nature of this problem and the changing operating conditions encountered in most scenarios suggested the use of model adaptation techniques. Another possible approach could be the use of nonlinear control. In particular Nonlinear Model Predictive Control (NMPC) is seen as a good candidate in order to keep the sub-optimality and the predictive behaviour particular to this technique.

4. The two-phase reactor considered was introduced as a simplification of the Tennessee Eastman problem. It would be interesting to extend the results found in this work to the original problem.

5. In this work the multivariable case for the MWA algorithm was obtained from the straightforward extension of the SISO case. It would be interesting to study in more detail to what extent this generalization is possible and to analyze theoretically the properties of this algorithm.

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APPENDIX

Table A.1: Transfer functions identified for the multivariable MPC

	u_1	u_2
F_4	$\frac{-1.62}{(0.8s+1)}$	$\frac{0.14\cdot(12.5s+1)}{(0.9s+1)(15s+1)}$
P	$\frac{47.96\cdot(7.6s+1)}{(14.9s+1)(0.25s+1)}$	$\frac{-44.293\cdot(-0.65s+1)}{(0.4s+1)(16s+1)}$
y_{A3}	$\frac{-0.71\cdot(-0.25s+1)}{(13.25s+1)(0.35s+1)}$	$\frac{1.62}{(13.5s+1)}$
liq	$g_{4.1}$	$\frac{0.32}{(13.5s+1)}$

Table A.1: Transfer functions identified for the multivariable MPC (continued)

	u_3	u_4
F_4	$\frac{-0.08\cdot(14.1s+1)}{(0.85s+1)(13.4s+1)}$	$\frac{-2.4s}{(0.003s+1)(0.8s+1)}$
P	$\frac{-10.42\cdot(2.2s+1)}{(16.65s+1)(0.3s+1)}$	$g_{2.4}$
y_{A3}	$\frac{0.08}{(16.3s+1)(0.25+1)}$	$\frac{-0.11s}{(s+1)(14s+1)}$
liq	$\frac{0.04\cdot(-7.6s+1)}{(16s+1)(1.2s+1)}$	$\frac{1}{(0.82s+1)}$

$$g_{4.1} = \frac{0.23\cdot(23.3s+1)}{(0.6s+1)(0.5s+1)(14.3s+1)}$$

$$g_{2.4} = \frac{12.5s}{(0.1s+1)(15s+1)} + \frac{1.3s}{(0.4s+1)(0.8s+1)}$$

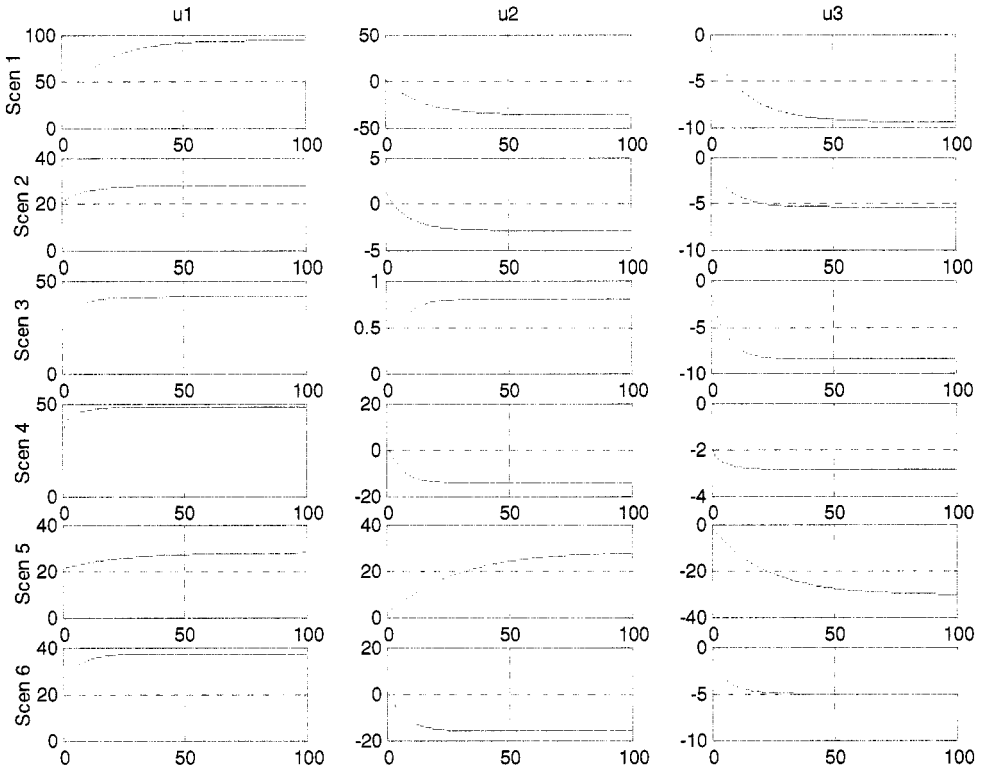

Figure A.1: Pressure responses at different conditions for unit steps on u_1, u_2 and u_3

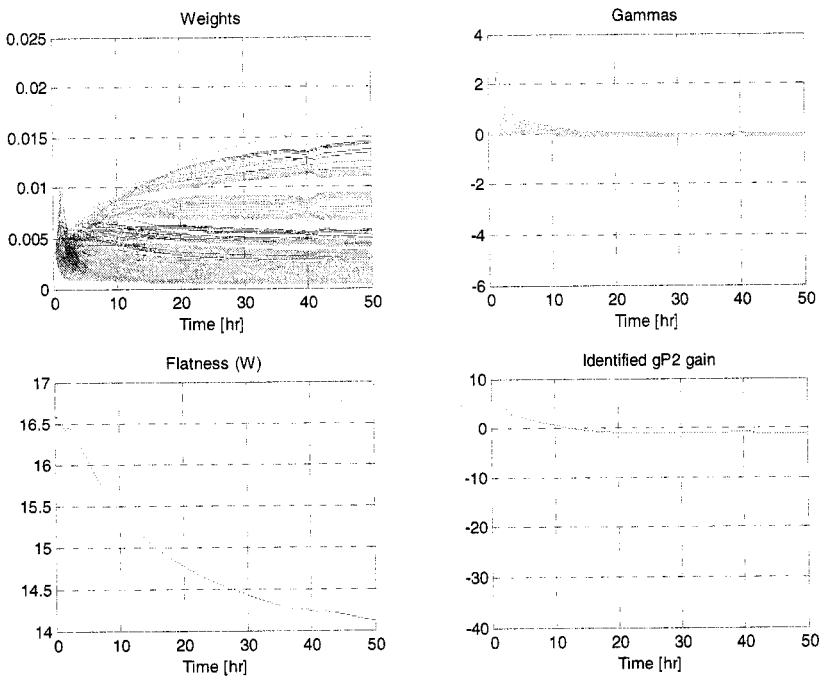

Figure A.2: Details on preliminary tests with SISO MWAC – Scenario 1

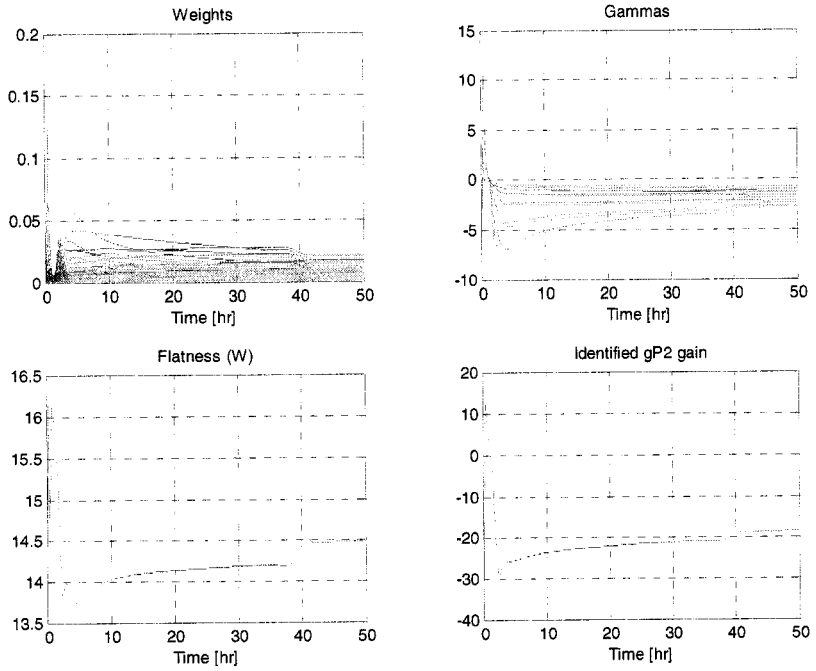

Figure A.3: Details on preliminary tests with SISO MWAC – Scenario 2

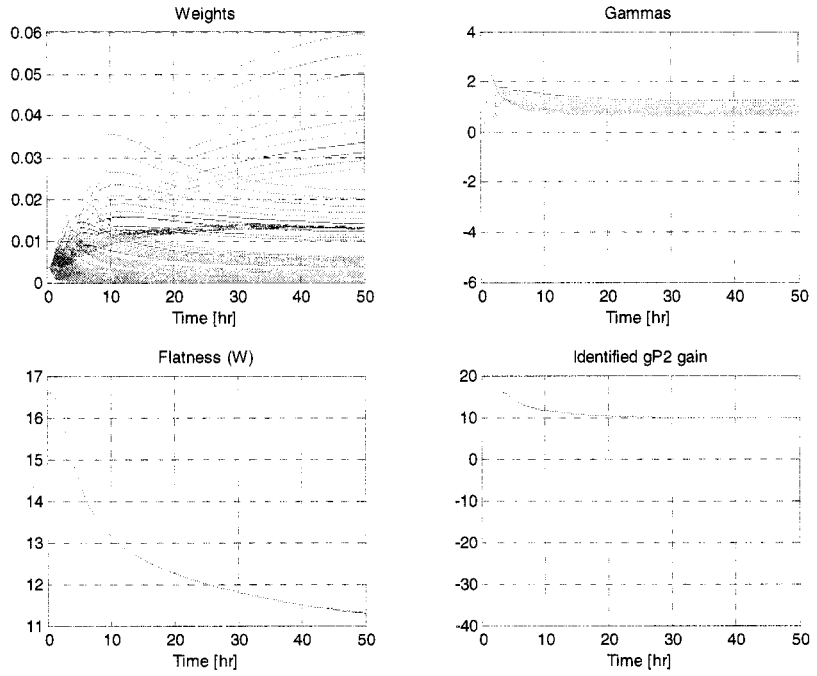

Figure A.4: Details on preliminary tests with SISO MWAC – Scenario 3

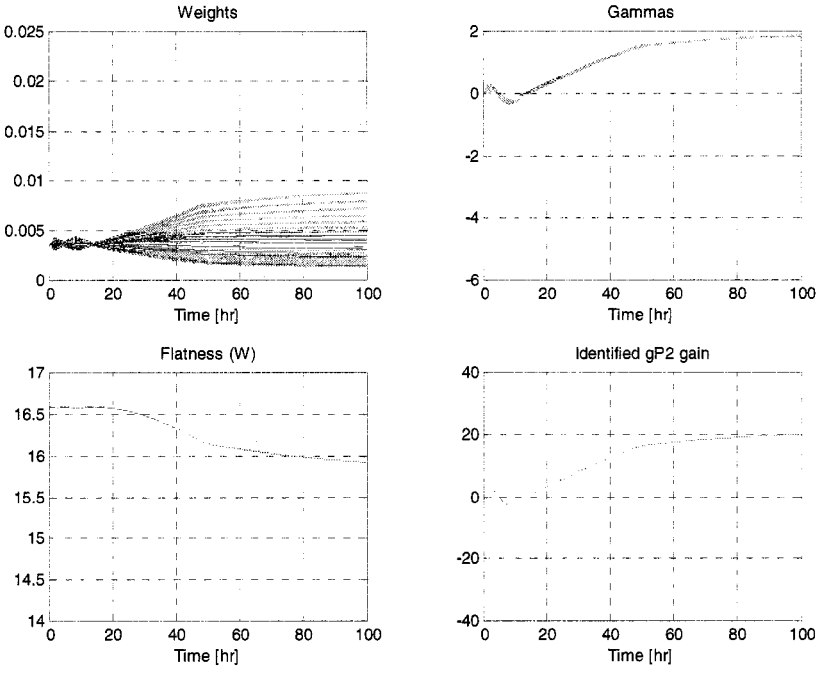

Figure A.5: Details on preliminary tests with SISO MWAC – Scenario 4

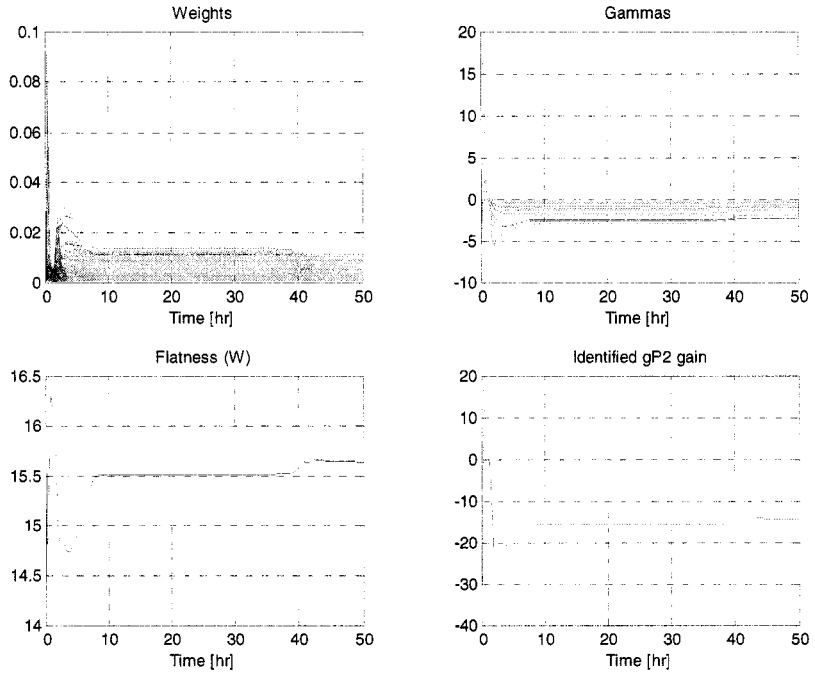

Figure A.6: Details on preliminary tests with SISO MWAC – Scenario 5

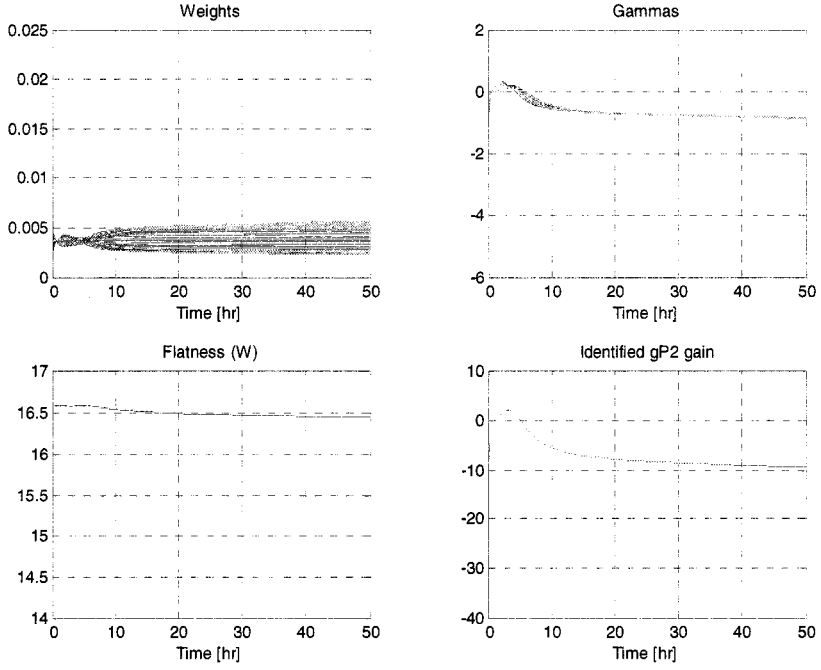

Figure A.7: Details on preliminary tests with SISO MWAC – Scenario 6

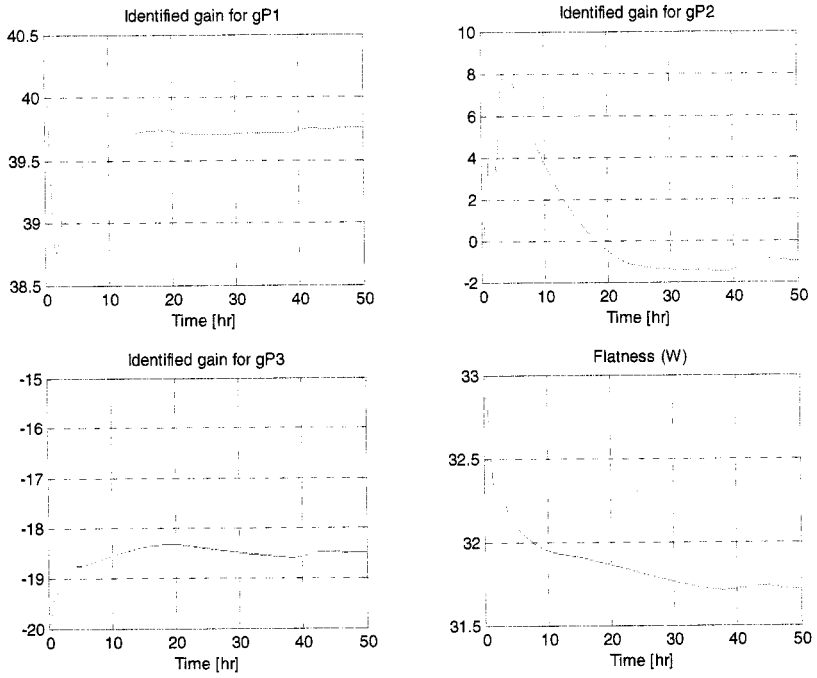

Figure A.8: Details on preliminary tests with MISO MWAC – Scenario 1

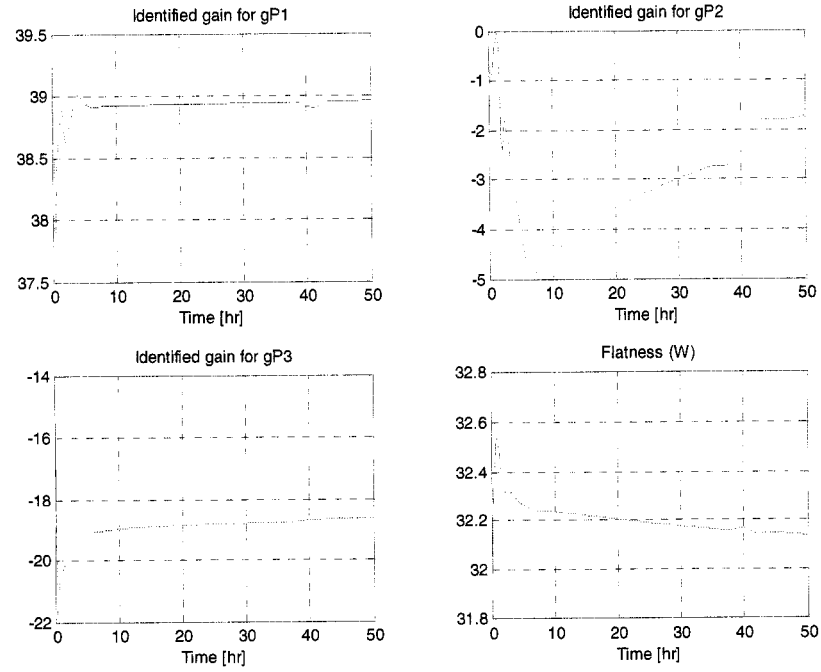

Figure A.9: Details on preliminary tests with MISO MWAC – Scenario 2

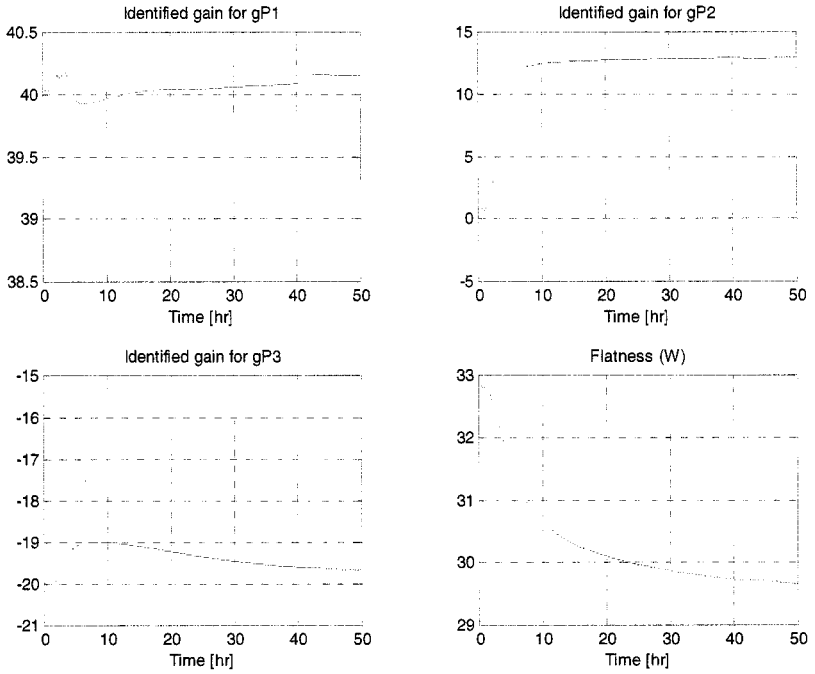

Figure A.10: Details on preliminary tests with MISO MWAC – Scenario 3

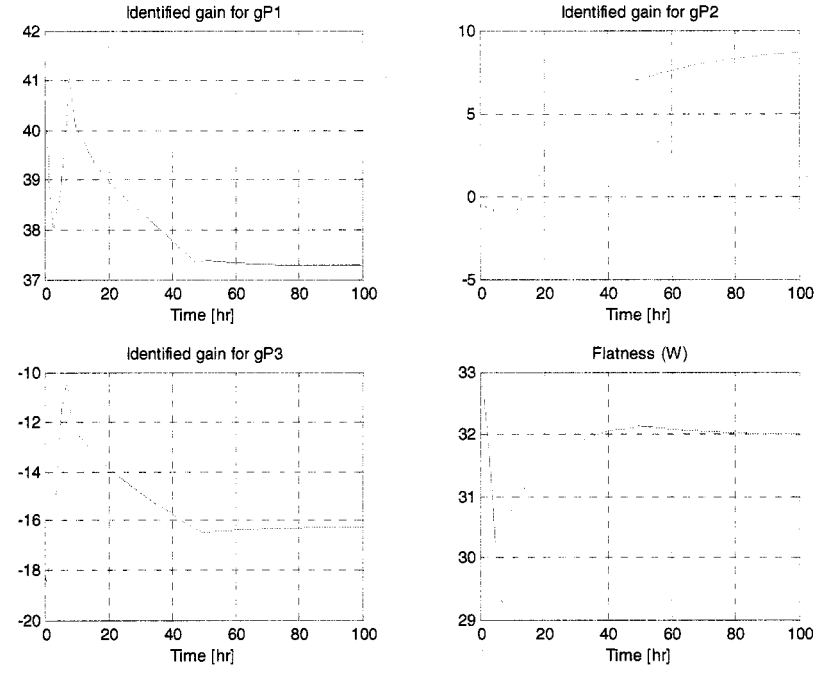

Figure A.11: Details on preliminary tests with MISO MWAC – Scenario 4

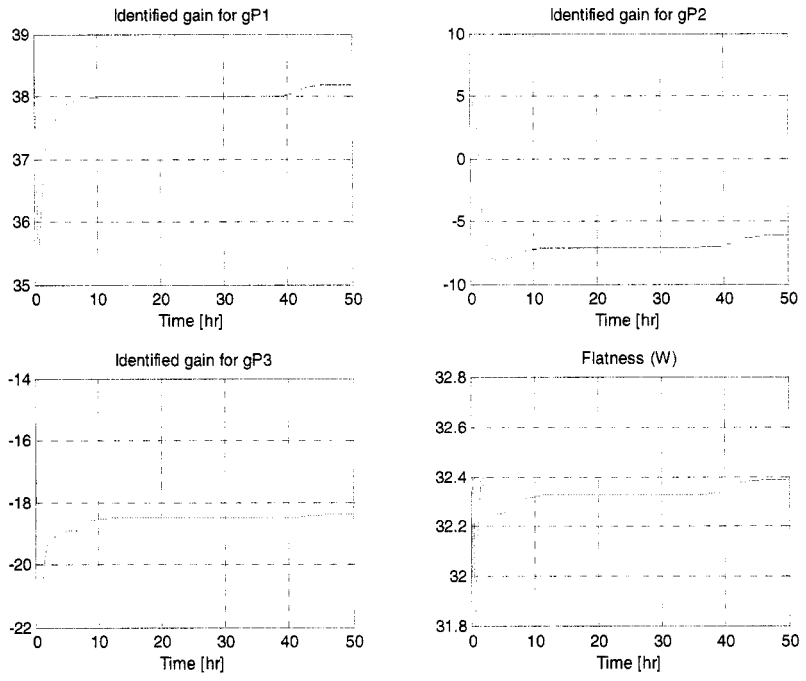

Figure A.12: Details on preliminary tests with MISO MWAC – Scenario 5

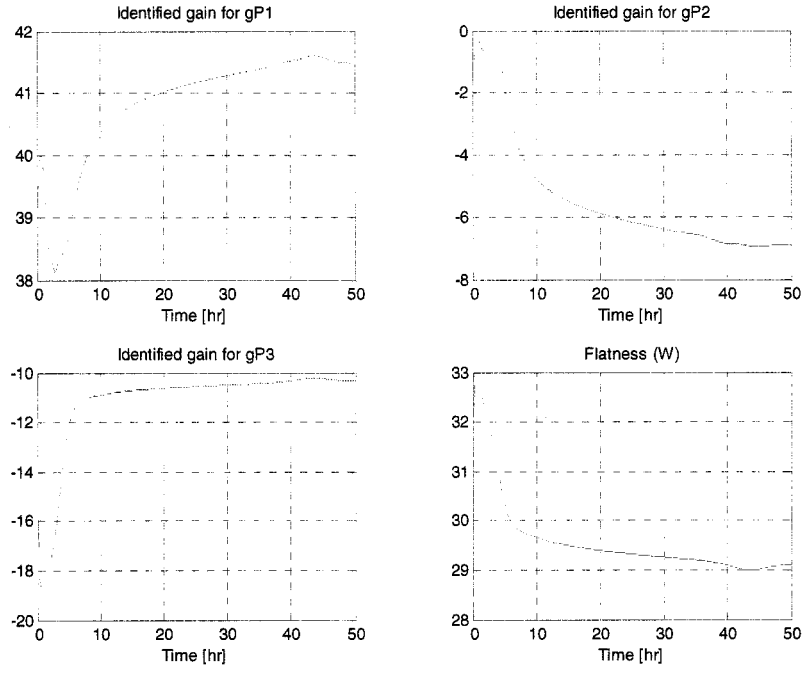

Figure A.13: Details on preliminary tests with MISO MWAC – Scenario 6

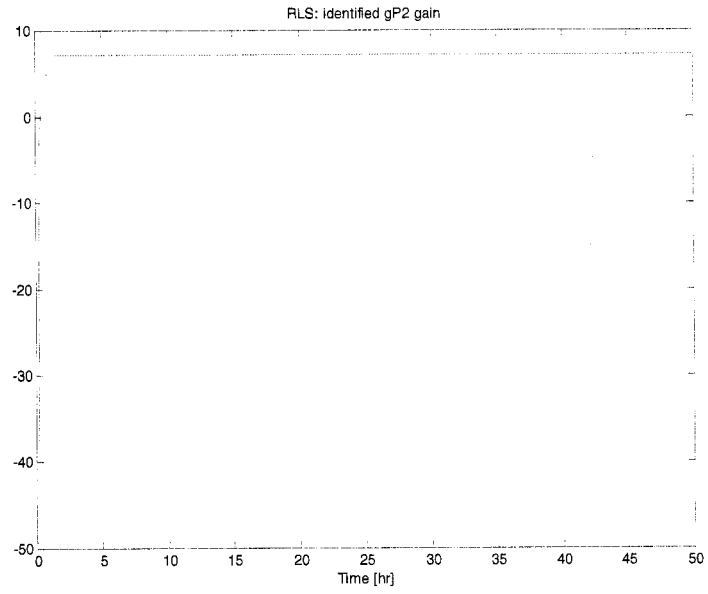

Figure A.14: Monvariable RLS approach – profile of identified K_{P2} – Scenario 1

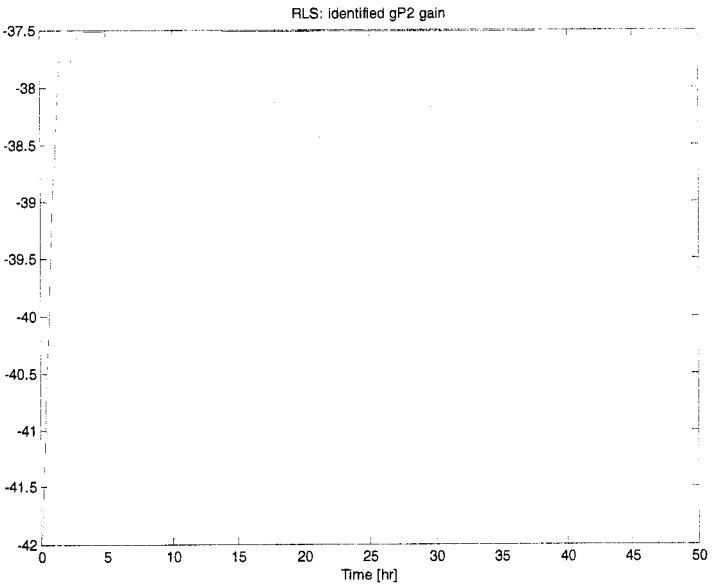

Figure A.15: Monvariable RLS approach – profile of identified K_{P2} – Scenario 2

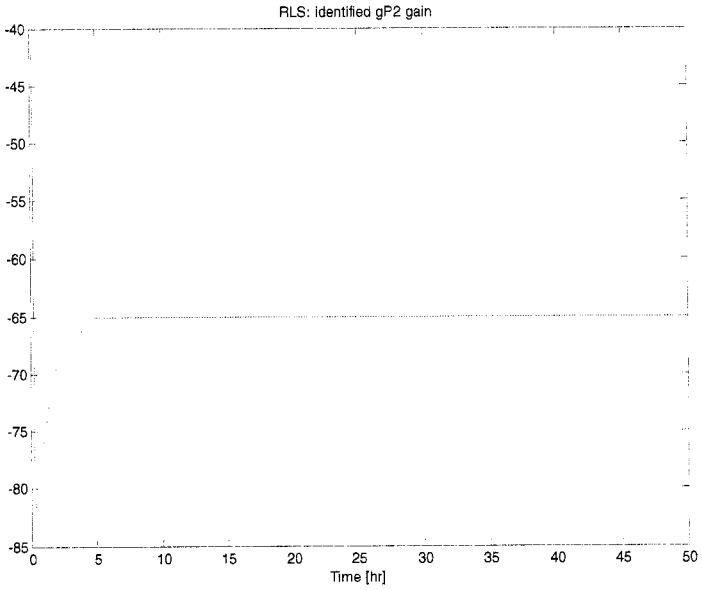

Figure A.16: Monvariable RLS approach – profile of identified K_{P2} – Scenario 3

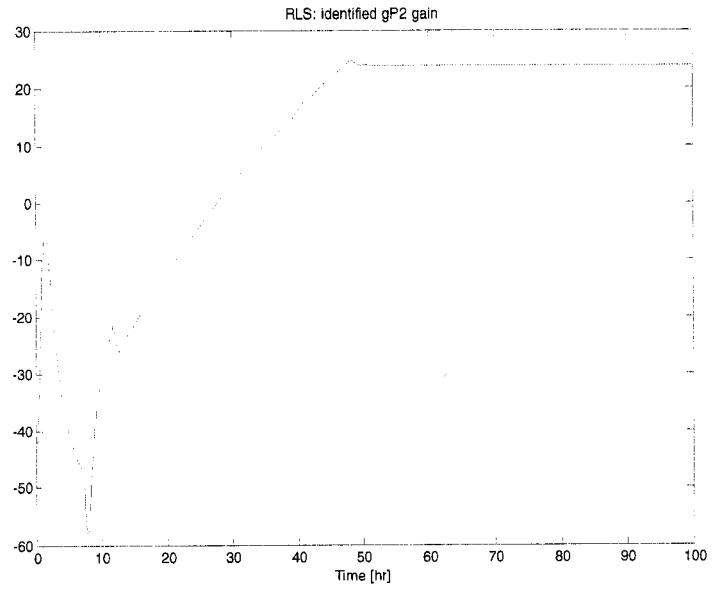

Figure A.17: Monvariable RLS approach – profile of identified K_{P2} – Scenario 4

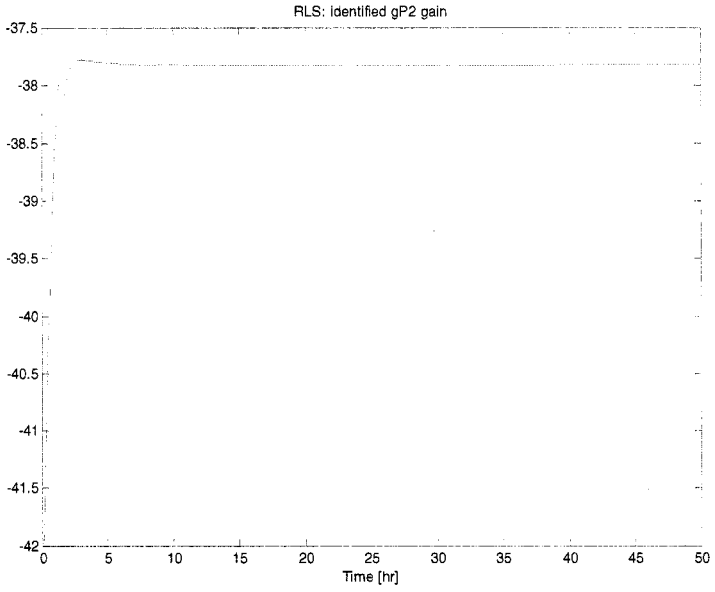

Figure A.18: Monvariable RLS approach – profile of identified K_{P2} – Scenario 5

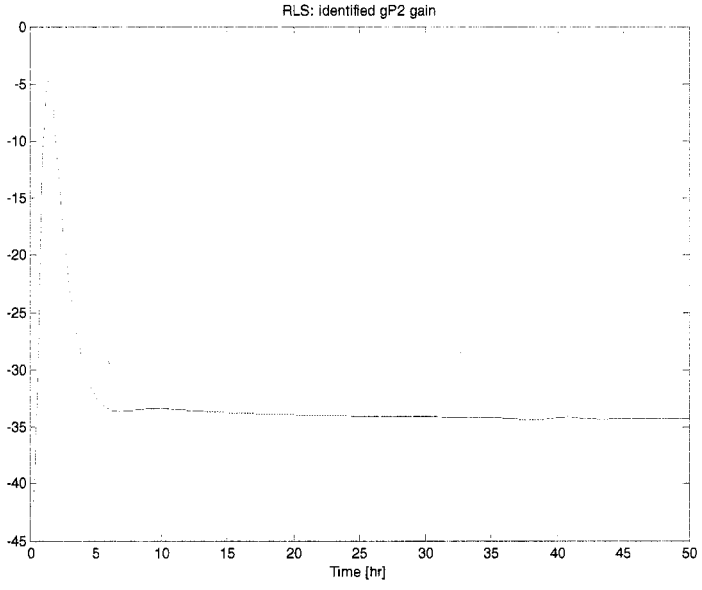

Figure A.19: Monvariable RLS approach – profile of identified K_{P2} – Scenario 6